Elastic properties of granular materials

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Elastic Properties of Granular Materials

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Signature of Author ....A. Paine..

A. C. Paine

God be in my head and in my understanding;

God be in my eyes and in my looking;

God be in my mouth and in my speaking;

God be in my heart and in my thinking;

God be at my end and at my departing.

Richard Pyson's *Horae B. V.M.* Sarum 1514

Summary

Granular materials consist of many components packed together with a complex microstructure of solid and fluid phases. A dense, random packing of spheres is one simple model that can be used to describe such a medium and which can help to predict its properties. This simplification has been used by many authors, including Walton [86] upon whose work this thesis is based. His work, along with relevant background material, is described in detail in Chapter 1. The work presented here concentrates on extending and developing Walton's model, which predicts the macroscopic properties of a packing of spheres, using the known microscopic properties of the grains. In particular, the effective elastic moduli for the packing are derived.

Chapter 2 extends Walton's model [86] to consider the effect of an initial biaxial compression applied to a packing of equal-sized spheres. The effective elastic moduli in this case are derived, first using precisely the same method as Walton and then also the results of Slade [76] who found that a modification to Walton's theory is required.

In Chapter 3, a perturbation of Walton's theory is considered in order to obtain modified expressions for the effective elastic moduli of a random packing of equal sized spheres. Chapter 4 then discusses the numerical calculations that must be carried out, in order to calculate the value of parameters which arise in the theoretical expressions of Chapter 3. At the end of Chapter 4, the values predicted by the new theoretical expressions are compared with those of a numerical simulation by Jenkins *et al.* [43]. Chapters 5 and 6 continue to develop Walton's method, extending the work to a binary packing of spheres, that is a random packing containing two sizes of sphere. Chapter 5 applies Walton's method directly, but in Chapter 6 a perturbation of this method is again used, thus combining the methods presented in Chapters 3 and 5.

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The work in Chapters 5 and 6 would not have been possible without the kind help of Dr Luc Oger of the Groupe Matiere Condensee et Materiaux, University of Rennes in France. His hours of work in order to obtain simulation results and his helpful comments, are much appreciated.

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Notation

For easy reference later on, presented here is a summary of the main notation used in this thesis.

$\mathbf{X}^{(n)}$ The position vector of the centre of the nth sphere.

$\mathbf{u}^{(n)}$ The displacement of the centre of the nth sphere.

$\omega^{(n)}$ The rotation of the nth sphere about an axis through its centre.

$\mathbf{F}^{(nn')}$ The force acting on the nth sphere due to its contact with the n'th.

$\mathbf{I}^{(nn')}$ The unit vector directed along the line of centres between the nth and n'th spheres, $\mathbf{I}^{(nn')} = \frac{\mathbf{X}^{(n)}-\mathbf{X}^{(n')}}{||\mathbf{X}^{(n)}-\mathbf{X}^{(n')}||}$

R is the sphere radius

N is the total number of of spheres within the packing.

V is the total volume of the packing.

$\eta^{(n)}$ is the average number of spheres in contact with the nth sphere, η is the average number of contacts within the packing.

ϕ is the volume concentration of the spheres, i.e. $\phi = \frac{4\pi R^3 N}{3V}$

$J_i^{(n)} = \frac{1}{\eta^{(n)}} \sum_{n'} I_i^{(nn')}$

$N_{ijk}^{(n)} = \frac{1}{\eta^{(n)}} \sum_{n'} I_i^{(nn')} I_j^{(nn')} I_k^{(nn')}$

$V_{ijkl}^{(n)} = \frac{1}{\eta^{(n)}} \sum_{n'} I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} I_l^{(nn')}$

From chapter 3 onwards, $< . >$ represents the average value within the packing, taken over all contacts.

$\alpha = \frac{1}{3} < I_i^{(nn')} J_j^{(nn')} >$

$\chi = \frac{1}{3} < N_{ijk}^{(nn')} I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} >$

$B = \frac{1}{4\pi} \left(\frac{1}{\mu} + \frac{1}{\lambda+\mu} \right)$, λ and μ are the Lamé moduli for the material

$C = \frac{1}{4\pi} \left(\frac{1}{\mu} - \frac{1}{\lambda+\mu} \right)$

$A = \frac{(2B+C)}{(14B+3C)}$

$R' = R_l R_s (R_l + R_s)^{-1}$, where R_l and R_s are the radii of large and small spheres, respectively.

Chapter 1

Introduction

1.1 Overview of Thesis

There has been an increasing interest in the study of granular materials over the past decade and a half. It has become a widely inter-disciplinary work area. A series of conferences entitled 'Powders and Grains' has brought together some of the various research advances from many different groups. The first held in Clemont-Ferrand, France, in 1989 [7] has been followed by a further two, one held at Aston in 1993 [80] and the most recent at Durham, North Carolina in 1997 [3]. They have concentrated on the subject of particulate ensembles and have shown the rapid increase in knowledge and the varied applications that are possible in many research areas.

Another specific example of a compilation of work is the book, 'Disorder and Granular Media', edited by Bideau and Hansen [8]. This contains recent progress that has been made in the physics of granular material as well as some fundamental concepts and ideas about the field, such as the geometrical characterization of granular media and elementary approach to flow in porous media. The book is intended to be accessible to researchers from a variety of backgrounds.

Granular materials are met in a large number of situations. For example, in materials science, they occur in the initial stage of preparation of composites, ceramics and sintered materials. Their various qualities are critically dependent upon the condition of the initial setting. In chemical engineering, many processes involve the use of finely divided matter, for example, anything from the combustion of solids, to heat exchangers and catalysers. Within agriculture and the food industry, the processes which make use of natural granular substances and powders of very different grades, depend upon the heterogeneous structure. Probably the subject areas in which the most research has been done are mechanical and soil engineering and also the geophysical sciences. Naturally occurring geological structures can be observed to exhibit many effects of packing and flow of grains. Civil engineering should also be mentioned, particularly in the use of grains of variable size, mixed with a bonding agent.

There is a growing interest in the use of numerical simulations to predict the properties of granular media. These have again been used in a wide variety of applications. One approach is that in which the granular material is treated as an ensemble of particles, rather than as a continuum. Cundall [19] was one of the first to introduce this technique and since then it has been applied to statistical micromechanics, Cundall and Strack [24] and Bathurst and Rothenburg [2], the constitutive behaviour of granular soils, analysis of rock-support interaction [50] and other areas of soil mechanics [81]. It was the results of numerical simulation which motivated most of the work presented in this thesis. There was an apparent lack of agreement between the predictions of the simulation and those of the theory.

This thesis contains the modelling of a granular material as a system of spherical particles and attempts to predict the macroscopic properties of this packing, from the known microscopic properties. We concentrate on finding the effective elastic moduli from the known properties of the grains which include elastic properties of each individual grain, the density of the packing and the type of contact between one grain and another. We concentrate specifically on spherical grains. When the particles are not spherical, particle shape is a further microstuctural known quantity, the effects of which will influence the overall behaviour. Several authors have considered non-spherical particles, including in particular Sackfield and Hills [69] and [70]. In his thesis, Slade [76], considered an oblique-oblique loading of two oblate spheroidal particles and then proceeded to use this to model a random packing of such particles. The purpose of his work was to attempt to model packings of shale particles such as might be present in an ocean bed.

As well as concentrating on spherical particles, we also specifically consider contacting particles which have identical elastic properties. Much work has been done on composite materials, for example, Hashin [37] provides a useful survey to review the analysis of composites from the perspectives of applied mathematics and engineering science. He considers the properties of three general types of composites: 1) statistically isotropic composites, this group includes the cases of random mixtures of two phases, matrix containing spherical type particles or randomly oriented elongated particles and porous media, 2) fiber composites, and 3)cracked materials.

The contact between two spheres is a fundamental problem which we shall consider. Chapter 2 is an extension of the work found in Walton [86]. When Walton [86], originally did the work he only considered the results for initial hydrostatic and uniaxial strains. Expressions for the effective elastic moduli are calculated upon application of a further general incremental strain. Our Chapter 2 considers the same calculations for a random packing of equal sized spheres under an initial applied compressive biaxial strain.

Chapter 3 proceeds to look at the uniform strain approximation, described later in this first Chapter and the method used by Walton [86] amongst others. In fact, we also use it in Chapter 2 to describe the displacement of each sphere after the strain has been applied to the boundary of the packing. Chapter 3, however, attempts to modify this approximation in order to obtain revised theoretical predictions of the elastic properties, when the average co-ordination number of the packing is fairly low. The effective elastic moduli are calculated and the results compared with the numerical results due to Jenkins *et al.* [43].

In Chapter 4, we discuss the numerical simulations performed in order to determine the values of those parameters which arise in the theoretical calculations. We briefly consider the results for 2-D packings although we are mainly concerned with those for 3-D. These parameter values allowed us to compare our new theoretical results from other chapters with previously obtained numerical simulation predictions.

Chapters 5 and 6 deal with a random binary packing of spheres, that is a random packing containing spheres of two different sizes. Chapter 5 incorporates the use of the uniform strain approximation, again in order to calculate the effective elastic moduli after considering initial hydrostatic, uniaxial and biaxial compressive strains. Chapter 6 combines the methods of both Chapters 3 and 5 to determine the effective elastic moduli using our perturbation of the uniform strain approximation, applied to a binary packing of spheres. Chapter 6 also contains a description of the numerical simulations

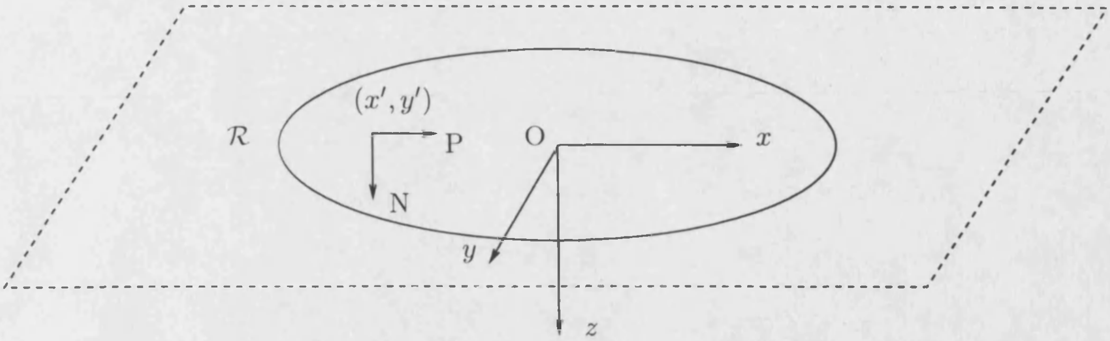

Figure 1-1: *The region $\mathcal{R}$ on the boundary of the half-space $z > 0$*

that were performed to calculate the values of parameters that arise in the theoretical expressions.

1.2 Contact Problems

We begin in this section by presenting several results which will be required later in the thesis when discussing the problem of two elastic spheres in contact. We initially consider the deformations that occur when a semi-infinite, elastically isotropic half-space is loaded under normal and tangential tractions. Outside the loaded area, both the normal and tangential forces are zero. In general, the solutions to these half-space problems can be used when considering Hertz [39] theory of elastic contact. Restricting attention to the particular case of a circular region of applied traction, this can be applied to the specific case of Hertz theory for two elastic spheres in contact.

1.2.1 Half-space Problems

Figure 1-1 shows the set of rectangular Cartesian axes $Oxyz$ which we shall consider, where the z-axis is directed downwards. The half-space $z > 0$ is bounded by the plane $z = 0$. Under the action of normal and tangential loadings, applied to the region $\mathcal{R}$, deformations and stresses are produced. As the loading is zero outside $\mathcal{R}$, we have a problem in which all the tractions are specified on the boundary $z = 0$. In the next sections we discuss the solutions of Boussinesq [11] and Cerutti [15], who use the theory of potentials to find the solutions to such problems.

Such solutions are often unique only to within an arbitrary rigid body displacement and rotation and thus we impose the condition that the displacement and rotation at infinity tend to zero.

1.2.2 Boussinesq's Problem

The problem of finding the surface displacements due to a concentrated normal force acting on the boundary of a homogenous isotropic half-space is known as Boussinesq's problem. Several books include the derivation of the potential function of Boussinesq [11] and also that of the potential function of Cerutti [15], this latter problem being described in the next section. Some such books include those written by Love [51], Mal and Singh [52] and Westergaard [90].

Here we do not present the derivation of the solutions, we simply list the results given by Walton [85] for a point force

$$N(x,y) = N_0\delta(x-x')\delta(y-y') \tag{1.1}$$

acting normally on the surface of the half-space $z > 0$, in the positive z-direction. N_0 is a constant and $\delta(.)$ is the Dirac delta function. This concentrated force acts at the point (x', y'), as shown in figure 1-1 and is of magnitude N_0. The surface displacements resulting from this force are

$$\begin{aligned} u_l(x,y) &= -\frac{(B-C)N_0X}{2S^2} \\ v_l(x,y) &= -\frac{(B-C)N_0Y}{2S^2} \\ w_l(x,y) &= \frac{BN_0}{S}. \end{aligned} \tag{1.2}$$

The displacements $u_l(x,y)$, $v_l(x,y)$ and $w_l(x,y)$ are the surface displacements in the x-, y- and z- directions respectively. We use the subscript l since when considering contact problems, these displacements will correspond to those of the lower half-space. The l, therefore, refers to a half-space with a positive z coordinate, that is, to the half-space $z > 0$. In the displacement expressions above we have defined local Cartesian coordinates $O'XY$, with origin (x', y'), as

$$X = x - x' \quad \text{and} \quad Y = y - y'. \tag{1.3}$$

The value of S is then determined by

$$S^2 = X^2 + Y^2 \tag{1.4}$$

and the elastic constants B and C are given by

$$\begin{aligned} B &= \frac{1}{4\pi}\left(\frac{1}{\mu} + \frac{1}{\lambda+\mu}\right) \\ C &= \frac{1}{4\pi}\left(\frac{1}{\mu} - \frac{1}{\lambda+\mu}\right) \end{aligned} \tag{1.5}$$

in terms of the Lamé moduli of the material, λ and μ. These may alternatively be written as

$$B = \frac{1-\nu^2}{\pi E},$$

$$C = \frac{\nu(1+\nu)}{\pi E}$$

in terms of Young's Modulus, E and Poisson's ratio, ν. Appendix D contains a table which shows the relationship between these and several other elastic constants.

1.2.3 Cerutti's Problem

Cerutti's problem [15], is similar to that of Boussinesq, except that we now consider a tangential concentrated force, acting in the positive x-direction on our half-space. This is described by

$$P(x,y) = P_0\delta(x-x')\delta(y-y'), \tag{1.6}$$

as shown in figure 1-1, where P_0 is a constant. The surface displacements that result from this applied force are given in Walton [85]. They are

$$\begin{aligned} u_l(x,y) &= (\frac{B}{S} + \frac{CX^2}{S^3})P_0 \\ v_l(x,y) &= \frac{CP_0XY}{S^3} \\ w_l(x,y) &= \frac{(B-C)P_0X}{2S^2} \end{aligned} \tag{1.7}$$

where $u_l(x,y)$, $v_l(x,y)$ and $w_l(x,y)$ represent the same directional displacements as in the previous section and X, Y, S, B and C are also defined as before.

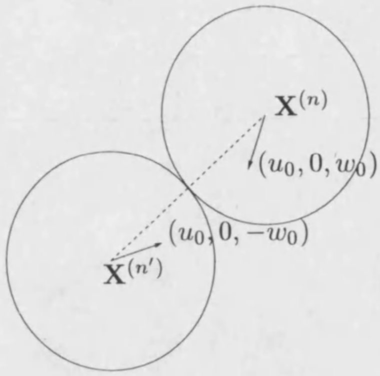

Figure 1-2: *Two Spheres Initially in Point Contact*

1.2.4 Distributed Normal and Tangential Loads

We can generalise the results quoted in the previous two subsections, to the situation where the stresses are due to distributed normal or tangential loads or both. Consider a general distribution of loading where $N(x,y)$ is the normal component of the traction and $P(x,y)$ and $Q(x,y)$ are the components of traction in the tangential x-and y-directions respectively, acting on the half-space $z > 0$. These can be thought of as a continuous distribution of point forces acting over part of the surface, in a region $\mathcal{R}$ and are zero outside this.

In the last two sections, we imposed the condition that the half-space have zero displacement at infinity. We now wish to impose a displacement $(u_0, 0, -w_0)$ at infinity on the half-space $z > 0$ and an equal and opposite one at minus infinity on $z < 0$. This will enable us to use our half-space results in the sphere contact problem. We shall see later, in section 1.2.7, that provided the contact area is small in relation to the size of each sphere, we can regard two contacting spheres as half-spaces thus applying the results from this section. When two spheres are compressed together, the relative displacements can be obtained by considering the displacement that the centre of the lower sphere undergoes, $(u_0, 0, -w_0)$ and the upper an equal and opposite one. Figure 1-2, shows two spheres initially in point contact.

Integrating the expressions given for the surface displacements, u, v and w, due to the force distributions N, P and Q over the whole region $\mathcal{R}$, equations (1.2) and (1.7) yield:

$$u_l(x,y) \quad = \quad u_0 + \int_{\mathcal{R}} \left(\frac{BP(x',y')}{S} + C\frac{[X^2 P(x',y') + XYQ(x',y')]}{S^3} \right.$$

$$
\begin{aligned}
& \qquad\qquad\qquad\qquad\qquad\qquad -\frac{(B-C)XN(x',y')}{2S^2}\Bigg)\, dx'dy' \\
v_l(x,y) &= \int_{\mathcal{R}} \left(\frac{BQ(x',y')}{S} + C\frac{[XYP(x',y') + Y^2Q(x',y')]}{S^3} \right. \\
& \qquad\qquad\qquad\qquad\qquad\qquad \left. -\frac{(B-C)YN(x',y')}{2S^2}\right) dx'dy' \\
w_l(x,y) &= -w_0 + \int_{\mathcal{R}} \left((B-C)\frac{[XP(x',y') + YQ(x',y')]}{2S^2} + \frac{BN(x',y')}{S} \right) dx'dy'
\end{aligned} \tag{1.8}
$$

For the particular problem that arises in the contact of two elastic spheres, the distribution of $N(x,y)$, $P(x,y)$ and $Q(x,y)$ acting on the lower sphere is equal and opposite to the traction that acts on the upper. Similarly, by integration, we can also obtain the total displacements acting on the upper sphere, $u_u(x,y)$, $v_u(x,y)$ and $w_u(x,y)$.

Walton [85], states that for the force distributions arising in the problem of contact of two spheres, the configuration would be identical whether viewed from the upper or lower sphere. For the case of displacement of the centre of the lower sphere having the form $(u_0, 0, -w_0)$, the following symmetries hold:

1. P and N are symmetric and Q is antisymmetric in both x and y and
2. u and w are symmetric and v is antisymmetric in y.

We define $u_+(x,y)$, the absolute displacement and $u_-(x,y)$, the relative displacement, as follows:

$$
u_+(x,y) = \frac{1}{2}(u_l(x,y) + u_u(x,y)) \quad \text{and} \quad u_-(x,y) = \frac{1}{2}(u_l(x,y) - u_u(x,y)) \tag{1.9}
$$

and similarly define $v_+(x,y)$, $v_-(x,y)$, $w_+(x,y)$ and $w_-(x,y)$. This allows us to decouple the displacement equations into integrals containing the effects of the normal force, N, only and those containing the effects of tangential loadings, P and Q, only.

$$
\begin{aligned}
u_+(x,y) &= u_0 + \int_{\mathcal{R}} \left\{ \frac{BP(x',y')}{S} + C\frac{[X^2P(x',y') + XYQ(x',y')]}{S^3} \right\} dx'dy', \\
v_-(x,y) &= \int_{\mathcal{R}} \left\{ \frac{BQ(x',y')}{S} + C\frac{[XYP(x',y') + Y^2Q(x',y')]}{S^3} \right\} dx'dy', \\
w_-(x,y) &= \frac{1}{2}(B-C)\int_{\mathcal{R}} \frac{[XP(x',y') + YQ(x',y')]}{S^2} dx'dy',
\end{aligned} \tag{1.10}
$$

and

$$\begin{aligned} u_-(x,y) &= -\frac{1}{2}(B-C)\int_{\mathcal{R}}\frac{XN(x',y')}{S^2}dx'dy', \\ v_+(x,y) &= -\frac{1}{2}(B-C)\int_{\mathcal{R}}\frac{YN(x',y')}{S^2}dx'dy', \\ w_+(x,y) &= -w_0 + B\int_{\mathcal{R}}\frac{N(x',y')}{S}dx'dy'. \end{aligned} \tag{1.11}$$

1.2.5 Pressure Applied to a Circular Region

In his book, Johnson [46], considers the surface displacement and stresses due to a pressure distributed over a circular region of radius a. He states that solutions in closed form can be found for axi-symmetrical pressure distributions of the form:

$$N(r) = N_0(1 - r^2/a^2)^n. \tag{1.12}$$

This is equation (3.27) of Johnson [46]. The coordinates (r, θ) are a system of plane-polar coordinates in the xy-plane sharing the common origin O (the xy-plane being as discussed in section 1.2.1). We only concern ourselves with two particular cases, $n = -1/2$ and $n = 1/2$, as these will be useful later in the problem of two spheres in contact. Johnson [46], however, also considers in detail the case $n = 0$.

Uniform Normal Displacement

We look first at the case $n = -1/2$ in equation (1.12), that is we consider a normal pressure of the form:

$$N(r) = \begin{cases} N_0(a^2 - r^2)^{-1/2}, & 0 \le r \le a \\ 0, & a < r \end{cases} \tag{1.13}$$

where N_0 is a constant and since we wish to apply these results to two spheres in contact, the region $\mathcal{R}$ is a circle of radius a and centred about O.

Johnson [46] shows that a pressure distribution of the form given in equation (1.13), causes a uniform normal displacement throughout the circular region of radius a, in the half space. This, therefore, would be the same pressure that would occur when a flat frictionless punch, of radius a, is pushed normally into an elastic half-space. The pressure at the edge of the punch is theoretically infinite.

We find the displacements in the normal direction, for this distribution and see that

$$\begin{aligned} w_l(x,y) &= \pi^2 B N_0 \\ w_u(x,y) &= 0. \end{aligned} \tag{1.14}$$

For a tangential traction of the same form, that is

$$P(r) = \begin{cases} P_0(a^2 - r^2)^{-1/2}, & 0 \leq r \leq a \\ 0, & a < r \end{cases} \tag{1.15}$$

the traction produces a uniform tangential displacement in the same direction as the traction itself. These resulting displacements are

$$\begin{aligned} u_l(x,y) &= \frac{\pi^2(2B + C)}{2} P_0 \\ u_u(x,y) &= 0. \end{aligned} \tag{1.16}$$

This type of tangential pressure distribution does not occur in the normal punch problem, but we will need the displacement results later on.

Hertz Pressure Distribution

We next consider the case when we have $n = 1/2$ in equation (1.12), that is a normal force distribution of the form

$$N(r) = \begin{cases} N_0(a^2 - r^2)^{1/2}, & 0 \leq r \leq a \\ 0, & a < r \end{cases} \tag{1.17}$$

where N_0 is again a constant and (r, θ) as in the previous subsection. This is the pressure given by the Hertz Theory, which in particular can be applied when we have two elastic spheres in contact.

According to Hertz theory, tangential tractions do not occur when bodies having the same elastic moduli are compressed together normally and the displacements resulting from this force are given by:

$$u_l(x,y) = -\frac{\pi N_0}{3}(B - C)x\frac{\{a^3 - (a^2 - r^2)^{3/2}\}}{r^2}$$

$$\begin{aligned} v_l(x,y) &= -\frac{\pi N_0}{3}(B-C)y\frac{\{a^3-(a^2-r^2)^{3/2}\}}{r^2} \\ w_l(x,y) &= \frac{\pi^2 N_0}{4}B(2a^2-r^2). \end{aligned} \tag{1.18}$$

Similarly, for a tangential distribution, in the x-direction of the form

$$P(r) = \begin{cases} P_0(a^2-r^2)^{1/2}, & 0 \le r \le a \\ 0, & a < r \end{cases} \tag{1.19}$$

where P_0 is a constant, the resulting displacements are found from integrals (1.10) to be

$$\begin{aligned} u_l(x,y) &= \frac{\pi^2 P_0}{4}(2B+C)a^2 - \frac{\pi^2 P_0}{16}\{(4B+C)x^2+(4B+3C)y^2\}, \\ v_l(x,y) &= \frac{\pi^2 P_0}{8}Cxy, \\ w_l(x,y) &= \frac{\pi P_0}{3}(B-C)x\frac{\{a^3-(a^2-r^2)^{3/2}\}}{r^2}. \end{aligned} \tag{1.20}$$

1.2.6 The Geometry of Surfaces in Contact

Before we examine Hertz theory for two spheres in contact, we consider the geometry of two non-conforming solids of general profile brought into contact. Johnson [46] also considers contact of conforming bodies which, using his definition, are contacts where the surfaces of the two bodies 'fit' together exactly or even closely without deformation. The non-conforming bodies we consider have dissimilar profiles and when initially brought into contact will touch at a point or along a line. They also have identical elastic properties, Gladwell [36], amongst others, discusses Dundurs' mismatch parameters that occur in the calculations for the contact of two materials which possess different elastic properties.

A theory of contact is required that will predict what happens to a point or line of contact when a load is applied to the configuration. But first, we examine the geometry of the problem. We take the point of contact of the two bodies as O, the origin of rectangular coordinate axes $Oxyz$. The z-axis is chosen to coincide with the common normal to the two surfaces at O and is directed into the lower solid. The xy-plane is then the tangent plane to the two surfaces. By choosing the orientation of x and y such that the term in xy vanishes, Johnson [46] approximates the profile of the lower surface as

$$z_1 = \frac{1}{2R_1'}x_1^2 + \frac{1}{2R_1''}y_1^2 \tag{1.21}$$

where R_1' and R_1'' are the principal radii of curvature on the surface at the origin. Also, using the same reasoning, the profile of the upper surface can be written as

$$z_2 = -\left\{\frac{1}{2R_2'}x_2^2 + \frac{1}{2R_2''}y_2^2\right\} \tag{1.22}$$

where the axes x_2 and y_2 may differ from x_1 and y_1. To find the separation between the surfaces, we need $h = z_1 - z_2$ and this can be written, relative to a common set of axes x and y, as

$$h = Ax^2 + By^2 + Cxy \tag{1.23}$$

where A, B and C are constants which depend upon the radii of curvature of the two surfaces. Again, choosing alternative axes so that C becomes zero, we have

$$h = Ax^2 + By^2 = \frac{1}{2R'}x^2 + \frac{1}{2R''}y^2. \tag{1.24}$$

In this case R' and R'' are defined as the principal relative radii of curvature. If the x_1 and x_2 axes are inclined at an angle θ to one another, in an appendix to his book, Johnson [46] shows that

$$\begin{aligned} A+B &= \frac{1}{2}\left(\frac{1}{R'}+\frac{1}{R''}\right) = \frac{1}{2}\left(\frac{1}{R_1'}+\frac{1}{R_1''}+\frac{1}{R_2'}+\frac{1}{R_2''}\right) \\ |A-B| &= \frac{1}{2}\left\{\left(\frac{1}{R_1'}-\frac{1}{R_1''}\right)^2+\left(\frac{1}{R_2'}-\frac{1}{R_2''}\right)^2\right. \\ &\qquad \left. +2\left(\frac{1}{R_1'}-\frac{1}{R_1''}\right)\left(\frac{1}{R_2'}-\frac{1}{R_2''}\right)\cos 2\theta\right\}^{1/2} \end{aligned} \tag{1.25}$$

and hence the values of A and B can be determined for a particular problem. At this point, for later convenience, we also introduce the equivalent radius, R_e, defined by

$$R_e = (R'R'')^{1/2} = \frac{1}{2}(AB)^{-1/2}. \tag{1.26}$$

From equation (1.24), it can be seen that the contours of constant gap h are ellipses whose axes are in the ratio $(B/A)^{1/2} = (R'/R'')^{1/2}$. For the particular example of two identical cylinders, each of radius R and with their axes inclined at 45°, we have

$R_1' = R_1'' = R$, $R_2' = R_2'' = \infty$ and $\theta = 45°$. Then equations (1.25), give $A+B = \frac{1}{R}$ and $B - A = \frac{1}{\sqrt{2}R}$ from which we have

$$A = \frac{1}{2R}\left(1 - \frac{1}{\sqrt{2}}\right), \quad B = \frac{1}{2R}\left(1 + \frac{1}{\sqrt{2}}\right). \tag{1.27}$$

The relative radii of curvature are, $R' = 1/2A = \sqrt{2}R/(\sqrt{2}-1)$ and $R'' = 1/2B = \sqrt{2}R/(\sqrt{2}+1)$ and the effective radius is thus:

$$R_e = (R'R'')^{1/2} = \sqrt{2}R. \tag{1.28}$$

In this thesis we shall deal with some problems relating to the contact between equal sized spheres of radius R. Hence we have, $R_1' = R_2' = R_1'' = R_2'' = R$ and $\theta = 0$, from which we find the values of A and B to be

$$A = \frac{1}{R}, \quad B = \frac{1}{R}. \tag{1.29}$$

However, the general geometry results will be useful later when we consider the contact of two spheres of different radii.

A cross-section of two bodies of general shape and elastic properties, is shown after the deformation, in figure 1-3. The initial configuration is not shown but we assume that the bodies were in point contact at O. Once a compression is applied (perpendicular to the common tangent of the two bodies), this causes a deformation in the neighbourhood of this original point of contact. If the bodies did not deform, they would overlap, as indicated by the dotted lines in the figure. A finite contact area therefore forms, which has purely normal tractions acting on it, provided the two bodies have identical elastic properties such as we wish to consider. If the elastic properties of the two bodies were different, tangential or shear tractions would occur which may cause the two surfaces to slip over each other.

We consider the configuration shown in the figure and the deformation that will occur in the vicinity of the point of initial contact, O, when a normal pressure is applied. A contact area will form that is small relative to the dimensions of the bodies. Points distant from the contact area, within the two bodies, will move parallel to the z-axis and approach each other by an amount $\delta_1 + \delta_2$. The displacement of the surface points

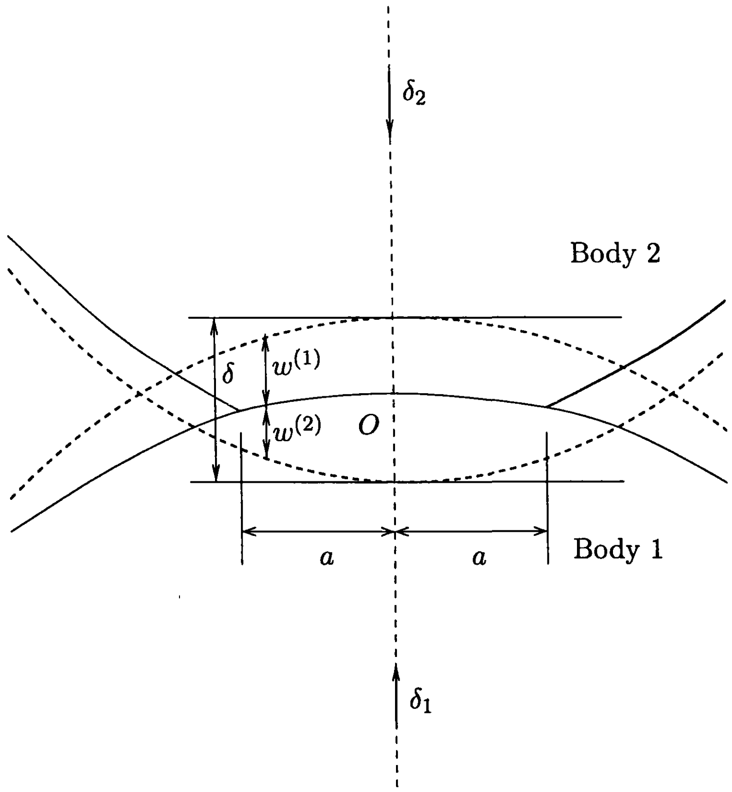

Figure 1-3: *Cross-Section of Two Non-Conforming Bodies in Contact*

within the contact area is $\delta_1 - w^{(1)}$, for the lower body and $\delta_2 - w^{(2)}$, for the upper one, where $w^{(1)}$ and $w^{(2)}$ are as shown in figure 1-3. Thus after the deformation, for points within the contact area, we have

$$w^{(1)} + w^{(2)} + h = \delta_1 + \delta_2 = \delta \tag{1.30}$$

where h is the initial separation of the two surfaces, as given in equation (1.24). For points that lie outside the contact area, they do not touch and so their displacements must satisfy:

$$w^{(1)} + w^{(2)} + h > \delta. \tag{1.31}$$

These last two equations, written in terms of the constants A and B give us

$$w^{(1)} + w^{(2)} = \delta - Ax^2 - By^2 \tag{1.32}$$

for the points within the contact area and

$$w^{(1)} + w^{(2)} > \delta - Ax^2 - By^2 \tag{1.33}$$

for those outside the contact area.

In the next section we turn to the theory of elasticity to show how the contact area, stress and deformation, might grow with increasing load.

1.2.7 Hertz Theory of Elastic Contact

Hertz [39] gave the first satisfactory analysis of the stresses at the contact of two elastic non-conforming solids. He formulated equations (1.32) and (1.33) which are satisfied by the normal displacements on the surface of the solid. He made the hypothesis that the contact area is in general elliptical and for simplification, approximated the elastic bodies as elastic half spaces.

In this thesis, the contacting bodies under consideration will be assumed to have the same elastic properties and to be isotropic. Johnson [46] also considers the contact of bodies of different elastic properties and the effects of anisotropy within the bodies is considered by Willis [91].

A number of assumptions are made in Hertz Theory. These are summarised in Johnson [46] and are given as the following:

- The surfaces are smooth, continuous and non-conforming;
- The strains are small;
- Each solid may be approximated by an elastic half-space for the purposes of relating surface tractions to surface displacements, on the contact area;
- The surfaces are frictionless.

These assumptions ensure that each body can be regarded as an elastic half-space, loaded over a small elliptical region on its surface. They also ensure that the strains in the contact area are sufficiently small to be within the scopes of the linear elasticity theory. Approximating the bodies by half spaces enables the results from Section 1.2.4 to be used and the boundary conditions are greatly simplified.

The elasticity problem in which we are interested, reduces to finding the normal pressure distributions acting over the contact area, which produce normal displacements of the surfaces satisfying equation (1.32), within the contact area and (1.33), outside it.

Johnson [46], considers Hertz theory for the general case of two solids of revolution in contact. We are particularly interested in the contact of two identical elastic spheres. Initially, the spheres are purely in point contact, but upon application of a force along the line of centres, a small contact area is formed. The contact area is circular for two solids of revolution and so will be circular in our particular case. Let the radius of this circle be a. We find the values of A and B from Section 1.2.6, these are

$$A = \frac{1}{R}, \; B = \frac{1}{R}. \tag{1.34}$$

The normal force causes a displacement w_0 of the centre of the lower sphere, along the line joining the two centres. Therefore, as the spheres are identical and have equal elastic moduli, we have $w_0 = \delta_1 = \delta_2$, so that $2w_0 = \delta_1 + \delta_2$. The surface displacements can also be written as $2w_+(x, y) = w^{(1)} + w^{(2)}$, where $w_+(x, y)$ is as given in equation (1.10) and $w_-(x, y) = 0$. The condition for contact (as in equation (1.32)) becomes

$$2w_+(x, y) = 2w_0 - \frac{x^2}{R} - \frac{y^2}{R}. \tag{1.35}$$

So, we must find the normal pressure distributions, acting on the contact area, that will produce a normal displacement as given. In addition, we must check that it satisfies the condition of no overlap outside the contact area.

We want to find $N(x, y)$, such that

$$B \int\int \frac{N(x', y')}{S} dx'dy' = 2w_0 - \frac{x^2}{R} - \frac{y^2}{R}. \tag{1.36}$$

One form of $N(x, y)$ that satisfies this requirement is as given below:

$$N(x, y) = \alpha(a^2 - r^2)^{\frac{1}{2}} \tag{1.37}$$

where α is constant for a particular sphere. From equation (1.18), we then have

$$B \int\int \frac{N(x', y')}{S} dx'dy' = \frac{\pi^2 \alpha B}{4}(2a^2 - r^2) \tag{1.38}$$

which when substituted into equation (1.36) yields

$$\frac{B\pi^2\alpha}{2}(2a^2 - r^2) = 2w_0 - \frac{r^2}{R}. \tag{1.39}$$

By equating coefficients of r^2 and the constant terms, then

$$\frac{B\pi^2 a^2\alpha}{2} = w_0 \tag{1.40}$$

and also

$$\frac{B\alpha\pi^2}{2} = \frac{1}{R}. \tag{1.41}$$

Now, solving for α and w_0 yields

$$\alpha = \frac{2}{\pi^2 RB} \tag{1.42}$$

and

$$a^2 = Rw_0. \tag{1.43}$$

Therefore, we can conclude that the normal traction distribution $N(x, y)$ is given by

$$N(r) = \frac{2}{\pi^2 RB}(a^2 - r^2)^{\frac{1}{2}} \tag{1.44}$$

and the radius of the Hertzian contact area, a, by

$$a^2 = Rw_0. \tag{1.45}$$

This solution has been shown to be unique (see Walton [85]).

1.2.8 The Oblique Compression of Two Elastic Spheres

As mentioned above, when two bodies with identical elastic properties are compressed together normally, no tangential tractions arise. Mindlin [57], considered a distribution of traction in which a tangential component is imposed, in addition to the normal force that is already acting in the problem. If there is infinite friction, then Mindlin [57], considering symmetry and continuity conditions, concludes that the normal component of traction is unaffected by the extra applied tangential loading, providing the spheres have identical elastic properties. Also, the displacements of the contact surface in the xy-plane correspond to a shift uniformly in the x-direction without change in shape or size. Equation (76) of Mindlin [57] gives the tangential traction across a circular contact area as:

$$P = \frac{P_1}{2\pi}(a^2 - r^2)^{-1/2}, \; r < a \tag{1.46}$$

with P_1 constant. This is clearly of the form seen in equation (1.15); that is, it is proportional to $(a^2 - r^2)^{-1/2}$.

Walton [85], considered the general case of the relative compression of two elastic spheres, so similarly to Mindlin [57], he looked at the Hertz problem but included a tangential loading. How these two papers differ is in the application of the loading. Walton [85] considers the more general oblique problem, where both normal and tangential displacements occur simultaneously, rather than separately. By decoupling the problem, as for the half space in Section 1.2.4, the solution to the normal and tangential components of the system can be found and thus we obtain the distribution (P, Q, N) on the contact area.

After the initial compression, the centre of the lower sphere has undergone a displacement $(u_0, v_0, -w_0)$ relative to the original contact point (the origin O) and the upper sphere an equal and opposite one. Thus a finite contact area is formed, with radius a. Using the notation of the previous section, Walton [86], gives the following expressions for the force exerted by the upper sphere on the lower sphere, in the case that the spheres are infinitely rough:

$$\begin{aligned} P_0 &= -\frac{4u_0}{\pi^2 R(2B+C)w_0}(a^2 - r^2)^{1/2}, \\ Q_0 &= -\frac{4v_0}{\pi^2 R(2B+C)w_0}(a^2 - r^2)^{1/2}, \\ N_0 &= \frac{2}{\pi^2 RB}(a^2 - r^2)^{1/2}. \end{aligned} \tag{1.47}$$

Mindlin and Deresiewicz [58] approach this problem by using a succession of incremental normal and tangential forces and then take the limit as these tend to zero, to obtain an approximation for the actual compression required.

Incremental Compression

Later in this chapter and those following, we wish to calculate the effective elastic moduli of a random packing of spheres. In order to do this, following the initial compression, a further incremental compression is applied. Walton [86] discusses the solution of this in which the centre of the lower sphere has undergone a further displacement $(\delta u_0, \delta v_0, -\delta w_0)$. The problem is solved for the two cases $\delta w_0 > 0$ (compression) and $\delta w_0 < 0$ (unloading) and if $\delta w_0 < 0$, then it is so small that contact is not lost. The new force distribution will have the form $(P_0 + \delta P, Q_0 + \delta Q, N_0 + \delta N)$ and we again decouple the governing equations to find the normal component. This is the same whatever the sign of δw_0 and is given by:

$$N_0 + \delta N = \frac{2}{\pi^2 RB}(b^2 - r^2)^{1/2}, \tag{1.48}$$

where b is the radius of the new circular contact area.

Considering initially the case where the spheres have an infinite coefficient of friction and taking the case $\delta w_0 < 0$ first, there can be no relative displacement of the two parts of the final contact surface and the tangential tractions arising have the form:

$$\begin{aligned} P_0 + \delta P &= K_1(a^2 - r^2)^{1/2} + K_2(a^2 - r^2)^{-1/2} \\ Q_0 + \delta Q &= L_1(a^2 - r^2)^{1/2} + L_2(a^2 - r^2)^{-1/2} \end{aligned} \tag{1.49}$$

the K_2 and L_2 terms being associated with the punch problem that we considered in Section 1.2.5. Walton [86] omits details of the calculations to find the constants K_1, K_2, L_1, L_2, however, we give a summary of these as the method is extended in Chapter 5 to the case of different sized spheres. We consider the displacement $u_-(x, y)$, as defined in Section 1.2.4, before and after the incremental compression. At the end of the initial compression this displacement on the contact area is given by equation (1.20)

$$u_-(x, y) = u_0 + \frac{\pi^2}{4}(2B + C)K_3 b^2 - \frac{\pi^2}{16}K_3\{(4B + C)x^2 + (4B + 3C)y^2\} \tag{1.50}$$

where

$$K_3 = \frac{4u_0}{\pi^2 R(2B + C)w_0} \tag{1.51}$$

which is the force constant from equation (1.47). The displacement after the incremental compression due to the distribution equation (1.49a) is found using equations (1.16) and (1.20). These give

$$u_-(x,y) = u_0 + \frac{\pi^2}{4}(2B+C)K_1a^2 + \frac{\pi^2}{2}(2B+C)K_2 - \frac{\pi^2}{4}K_1\{(4B+C)x^2 + (4B+3C)y^2\}. \tag{1.52}$$

As we have imposed a no-slip condition on the problem, this displacement must be the same as the displacement at the end of the initial compression. Equating coefficients of x^2 and y^2 and matching constant terms we see that

$$\begin{aligned} K_3 &= K_1 &(1.53)\\ u_0 + \frac{\pi^2}{4}(2B+C)K_3b^2 &= u_0 + \delta u_0 + \frac{\pi^2}{4}(2B+C)K_1a^2 + \frac{\pi^2}{2}(2B+C)K_2. \end{aligned}$$

Solving for K_1 and K_2, equations (1.48) and (1.49) become

$$\begin{aligned} P_0 + \delta P &= \frac{2}{\pi^2 R(2B+C)w_0}\{2u_0(b^2-r^2)^{1/2} + (a^2u_1 - b^2u_0)(b^2-r^2)^{-1/2}\},\\ Q_0 + \delta Q &= \frac{2}{\pi^2 R(2B+C)w_0}\{2v_0(b^2-r^2)^{1/2} + (a^2v_1 - b^2v_0)(b^2-r^2)^{-1/2}\},\\ N_0 + \delta N &= \frac{2}{\pi^2 RB}(b^2-r^2)^{1/2}. \end{aligned} \tag{1.54}$$

where b $(< a)$ is the radius of the new contact area and satisfies

$$b^2 = R(w_0 + \delta w_0) \tag{1.55}$$

and $u_1 = u_0 + \delta u_0$, $v_1 = v_0 + \delta v_0$. The radius of each sphere is R and the moduli B and C are as previously defined in terms of the Lamé moduli.

When $\delta w_0 > 0$ the contact area increases and as we again have no relative displacement of the upper and lower parts of the original contact surface, a similar condition will apply to the final contact surface. Walton [85] shows that this condition plus an energy flux argument are sufficient to ensure a unique solution. Considering the distribution

$$\begin{aligned} P_0 + \delta P &= K_1(b^2-r^2)^{1/2} + K_2(a^2-r^2)^{1/2}\\ Q_0 + \delta Q &= L_1(b^2-r^2)^{1/2} + L_2(a^2-r^2)^{1/2}, \end{aligned} \tag{1.56}$$

with $N_0 + \delta N$ as before, we calculate the displacements as above and matching them in the same way, we see that the force distribution is now given by

$$\begin{aligned}
P_0 + \delta P &= \frac{4}{\pi^2 R^2 (2B+C) w_0 \delta w_0}\{(b^2 u_0 - a^2 u_1)(a^2 - r^2)^{1/2} \\
&\qquad + (u_1 - u_0) a^2 (b^2 - r^2)^{1/2}\}, \\
Q_0 + \delta Q &= \frac{4}{\pi^2 R^2 (2B+C) w_0 \delta w_0}\{(b^2 v_0 - a^2 v_1)(a^2 - r^2)^{1/2} \\
&\qquad + (v_1 - v_0) a^2 (b^2 - r^2)^{1/2}\}, \\
N_0 + \delta N &= \frac{2}{\pi^2 RB}(b^2 - r^2)^{1/2}. \qquad (1.57)
\end{aligned}$$

Slade [76], extends these results for the oblique compression of two elastic spheres to include the effects of a non-zero value of the coefficient of friction. He also considers the oblique compression of two spheroidal particles.

Results for the Oblique Compression Problem

In the sections above we looked at the problem of the oblique compression of two elastic spheres as presented in Walton [85]. The spheres are now pressed together in such a manner that the centre of the lower sphere undergoes a displacement $(u_0, v_0, -w_0)$, during the initial deformation and the upper sphere an equal and opposite one, that is $(-u_0, -v_0, w_0)$. Following this, in the incremental stage the centre of the lower sphere undergoes a further displacement $(\delta u_0, \delta v_0, -\delta w_0)$ and the centre of the upper one $(-\delta u_0, -\delta v_0, \delta w_0)$. Considering first the case when friction has an infinite value, the total force acting across the contact area is found by integrating the distributions given in equations (1.47). Hence, we have

$$\overline{P}_0 = \frac{8u_0(Rw_0)^{1/2}}{3\pi(2B+C)}, \ \overline{Q}_0 = \frac{8v_0(Rw_0)^{1/2}}{3\pi(2B+C)} \qquad (1.58)$$

and

$$\overline{N}_0 = \frac{4R^{1/2}w_0^{3/2}}{3\pi B}. \qquad (1.59)$$

The constants B and C are defined in equation (1.5) in terms of the Lamé moduli and R is the radius of each sphere. For the incremental stage, two cases were considered in section 1.2.8. For $\delta w_0 < 0$, integrating equations (1.54), over the contact area yields the total incremental force acting, these are equation (2.10) of Walton [86]:

$$\overline{\delta P} = \frac{4}{3\pi R(2B+C)w_0}\left\{3a^2 b\delta u_0 - (a-b)^2(2a+b)u_0\right\},$$

$$\begin{aligned}\overline{\delta Q} &= \frac{4}{3\pi R(2B+C)w_0}\left\{3a^2b\delta v_0 - (a-b)^2(2a+b)v_0\right\},\\ \overline{\delta N} &= \frac{4(b^3-a^3)}{3\pi RB}.\end{aligned} \tag{1.60}$$

For the second case, if $\delta w_0 > 0$, equation (2.12) of Walton [86] gives us the total force acting this time, found by integrating equations (1.57)

$$\begin{aligned}\overline{\delta P} &= \frac{8(b^3-a^3)\delta u_0}{3\pi R(2B+C)\delta w_0},\\ \overline{\delta Q} &= \frac{8(b^3-a^3)\delta v_0}{3\pi R(2B+C)\delta w_0},\\ \overline{\delta N} &= \frac{4(b^3-a^3)}{3\pi RB}.\end{aligned} \tag{1.61}$$

Notice that $\overline{\delta N}$ is the same in both cases. The radii a and b satisfy the Hertz relationships

$$a^2 = Rw_0 \tag{1.62}$$

and

$$b^2 = R(w_0 + \delta w_0). \tag{1.63}$$

In general, the two sets of equations (1.60) and (1.61) will give different results for the incremental forces, but in the case of an infinitesimal increment they both reduce to

$$\overline{\delta P} = \frac{4(Rw_0)^{1/2}\delta u_0}{\pi(2B+C)}, \quad \overline{\delta Q} = \frac{4(Rw_0)^{1/2}\delta v_0}{\pi(2B+C)} \tag{1.64}$$

and also

$$\overline{\delta N} = \frac{2(Rw_0)^{1/2}\delta w_0}{\pi B}. \tag{1.65}$$

These are the results for infinitely rough spheres.

The results for the case of perfectly smooth spheres are also listed in equations (2.15) of Walton [86]. As there will be no shear traction across the contact area, then the total force acting at the end of the initial deformation will be

$$\overline{P} = \overline{Q} = 0, \quad \text{and} \quad \overline{N} = \frac{4R^{1/2}w_0^{3/2}}{3\pi B} \tag{1.66}$$

and the incremental forces will be

$$\overline{\delta P} = \overline{\delta Q} = 0, \quad \text{and} \quad \overline{\delta N} = \frac{2(Rw_0)^{1/2}\delta w_0}{\pi B}. \tag{1.67}$$

1.3 Granular Media

In their book, Wang and Nur [89], bring together a range of theories that are used to predict the elastic properties of granular media. The first chapter of the book summarises some frequently used theories and models of elastic properties of effective media that are applicable in particular to rocks. However, this is not the only application of the theory, it is of interest to many research fields including material sciences and seismic exploration. The book is split into several chapters but the introductory chapter summarises them within just four areas. These are:

- I. Effective Medium Theories
- II. Wave Propagation and Self-Consistent Theories
- III. Contact Theories
- IV. Anisotropy.

We are purely interested in the first and third of these and principally with the third. However, below is a brief summary of each of these areas, before we focus upon contact models and how we can bring together the results from the previous section to say something about the properties of some types of granular media.

Effective Medium Theories

A lot of effective medium theories were developed to study the elastic properties of composite materials such as cracked solids, porous media and multicomponent composite materials. One of the ways in which the properties of these materials can be determined is the method used by Wood [93], where the averaging is done by taking the sum of individual phase properties, weighted by their proportion of the total volume fraction of the medium. Other methods include using an upper bound on the effective elastic moduli found by Voigt [83], whilst studying an aggregate of crystals. This assumes that the strain is uniform throughout the aggregate. Reuss [68], also found a bound on the moduli but this time a lower one by assuming that the stress is uniform throughout the medium. Since Voigt's and Reuss' models only give upper and lower bounds, Hill [40] suggested taking the average of these two solutions. This does not have any physical meaning but gives an approximate value for the effective moduli. Voigt's and Reuss' models often provide the highest upper bound and lowest lower bound respectively for the effective moduli and so are not very practical. Hashin and Shtrikman [38], however, using a variational approach, derived improved upper and lower bounds for the effective moduli of multiphase materials. They claim that the bounds calculated are the least upper bound and the highest lower bound, derived when only the phase moduli and volume fractions are known. In the limiting case of the highest upper bound and lowest lower bound, they recover Voigt and Reuss' results respectively.

Wave Propagation and Self-Consistent Theories

Two of the most widely used theories for modelling the effect of fluid saturation upon seismic velocities within rocks are those of Gassmann [35] and Biot [9] and [10]. Walton and Digby [88] also consider a medium saturated with fluid. The Gassmann equation is only valid at low frequencies, at higher frequencies some of the assumptions break down. Biot developed his theory to cover the whole frequency range. Kuster and Toksoz [49] have derived a more general model to describe the wave velocity for a continuum with inclusions. Wang and Nur [89] discuss in some detail the work contained in these five papers. They also discuss three self-consistent theories, including that of Hill [40] who developed his self-consistent theory for spherical inclusions.

Contact Theories

Contact theories are used mostly for studying the elastic properties of granular media, as they will be in this thesis. As we have already seen, there are several theories to describe the interaction between individual grains in the form of spheres. Both the work of Hertz [39], for the application of a normal compressive force between two spheres and Mindlin [57] who considers several initial loadings of the spheres, have been described previously in this chapter.

Modelling the grains as spheres is one approach to the problem and many authors have chosen to do this. Some have considered regular packings, while others random packings. In Section 1.3.1 we discuss the random packing model presented by Walton [86] as this will be further developed in other chapters. Slade [76] also considered random packings, but discussed the results for a packing of oblate spheroidal particles. The motivation for this was the application of the results to shale-like rocks which are made up mostly of clay, in the form of flat, plate-like particles. Other minerals are present in the shale but it is the clay that is the load bearing part and thus will have the largest effect on the elastic properties of the shale. In general, elastic properties of shale are anisotropic and Hornby *et al.* [41] have also done some work to predict the effective elastic properties of shales using spheroids. Their theory is based upon a different approach to that of Slade, they use a combination of self consistent (SCA) and differential effective medium (DEM) approximations. Another approach is considered by Marion *et al.* [53], they modelled the shale as an isotropic elastic solid. They justified this from the experimental work of McGeary [55], who showed that the packings of binary mixtures depend upon the diameter ratio of the particles. For large diameter ratios, typically around 100, the mixture packing is close to ideal. That is, the small spheres do not affect the packing of the large and vice-versa. In the sand-shale model the diameter ratio is normally greater than 50.

Anisotropy

For the random packings of spheres such as we shall consider in this thesis, the effective medium is only anisotropic upon application of a uniaxial loading. However, it is clear that in rock samples this will not be the case as there may be cracks, for example, which result in anisotropy. Even if these cracks were randomly distributed through the medium, the application of uneven or directional strains to the rock would give anisotropic effective elastic constants. The papers within Wang and Nur [89] discuss this in more detail.

1.3.1 The Effective Elastic Moduli of a Random Packing of Spheres

In his paper, Walton [86] considers the calculation of the effective elastic moduli of a dense random packing of spheres. Other authors have also considered this calculation, however many of them consider regular packings, for example, Duffy [31], Duffy and Mindlin [32], Deresiewicz [27] and Walton [84]. Brandt [12] did consider a random packing, as did Digby [28]. However, Brandt [12] only looked at the effective bulk modulus and Digby [28] assumed that the spheres were bonded together (we shall see how this bonding affects his results, as compared with those of Hertz, in the next section).

The methods presented in Walton [86] will be used extensively in this thesis, and so in this section we present the main results and techniques. In our later work, we extend the initial conditions and modify the main assumption of uniform strain for the displacement of the sphere centres, as made in the paper. Chapter 2, looks at a different initial loading, Chapter 3 attempts to provide reasons why the numerical values given for the effective elastic moduli from the work of Walton [86], are so different from those found by experiment and numerical simulation. Chapters 5 and 6 continue along this path of thought and calculate the effective moduli in the case of a binary packing of different sized spheres.

We assume that the random packing of spheres occupies a large volume. It is a random packing in the sense that contact points are distributed with equal probability over the surface of each sphere. The spheres are all identical in that they are the same size and have the same elastic moduli. The sphere material is homogeneous and elastically isotropic. In the initial state, the spheres are in point contact with several of their neighbours. In theory, this could be as many as twelve but on average, for a dense packing, will be around eight or nine. When a confining strain is applied to the medium, this prevents separation of any spheres already in contact and creates small contact areas between neighbouring spheres. We assume, for simplicity, that no new contacts are formed during this process. Endres article [34], is an example of how the effects of contact generation can be considered within the model. The procedure for calculating the effective moduli is to then impose a further incremental strain on the material, that is one of much lower order than the original strain. The effective moduli are then determined from the relationship connecting the average incremental stress to the average incremental strain.

Alternatives to the Hertz Theory With Tangential Loading

Several other authors since Hertz [39] have also considered the problem of describing the contact area formed when two identical spheres come into contact. In a recent paper, Norris and Johnson [60] consider the incremental relation between the forces and displacements of the form:

$$\delta N = D_n(w_0)\delta w_0, \quad \delta T = D_t(w_0)\delta u_0 \tag{1.68}$$

where the force has been decoupled into its normal component δN and its tangential component δT and where D_n and D_t are the contact stiffnesses in the notation of Digby [28] and Winkler [92]. These take the form

$$D_n = C_n a_n(w_0), \quad D_t = C_t a_t(w_0) \tag{1.69}$$

where C_n and C_t are actual stiffnesses,

$$\begin{aligned} C_n &= \frac{4\mu}{1-\nu} = \frac{8\mu(\lambda+\mu)}{\lambda+2\mu}, \\ C_t &= \frac{8\mu}{2-\nu} = \frac{16\mu(\lambda+\mu)}{3\lambda+4\mu} \end{aligned} \tag{1.70}$$

and λ and μ are the Lamé constants for the spheres and ν is Poisson's ratio. The lengths a_n and a_t do not depend on the material properties of the spheres, but do depend on the type of contact. Several models are summarized in table 1 of Norris and Johnson [60] and are reproduced below.

Contact Model	Description	$a_n(w)$	$a_t(w)$ (a)	$a_t(w)$ (b)
I	Hertzian Contact	$(Rw_0)^{1/2}$	0	a_n
II	Initial Contact Radius b (Digby)	$\left[(R^2w_0^2 + \frac{b^4}{2})^{1/2} + \frac{b^2}{2}\right]^{1/2}$	b	a_n
III	Frictional Sliding (Mindlin and Dereseiwicz)	$(Rw_0)^{1/2}$	$\left(\frac{\theta}{a_n} + \frac{1-\theta}{c}\right)^{-1}$	

In all these models, the two sub-cases (a) and (b), correspond to (a) smooth contact with reversible slip; and (b) rough contact with no subsequent slip.

Mindlin and Deresiewicz' model

Mindlin and Deresiewicz wrote several papers analysing the mechanics near the contact region of two spheres, Mindlin [57], Mindlin and Deresiewicz [58] and Deresiewicz [26] and [27]. These extend the theory of Hertz to include tangential loading and oblique contact. The second of these papers concludes that the changes in traction and displacements depends not only upon the initial loading, but also upon the entire past history of the medium and the instantaneous relative change of tangential and normal forces.

Consider two spheres under a compressive load, N_0, resulting in a contact area of radius a. Expressions are found for a and for the normal displacement w. Now, an oblique force is applied with a tangential component T and a total normal force N. The additional force is applied incrementally and

$$\frac{dT}{dN} = \beta > f \tag{1.71}$$

where β is constant and f is the coefficient of friction between the sphere surfaces. Defining

$$\theta = \frac{f}{\beta} \quad \text{and} \quad c = (1 - T/fN)^{1/3}a, \tag{1.72}$$

the expressions found by Mindlin and Deresiewicz [58] for the normal and tangential compliances of the spheres can be expressed in terms of the notation of Norris and Johnson [60], as shown in the table above. If the spheres are perfectly smooth, then $c \equiv 0$ and we have no tangential tractions acting across the contact area. Thus the conclusions are identical to those of the Hertz theory (case Ia in the table). If the friction is infinite or $\theta = 1$ then we recover the results of Walton [86], as described in the next section.

Digby's Model

Digby [28], modelled porous granular rock as a random packing of identical spheres, bonded together across small areas before the initial loading is applied. This initial contact area is circular and has radius b. Upon application of a compressive normal force N, acting on the particles, the contact area increases, having a new radius a which is given by:

$$a(a^2 - b^2)^{1/2} = Rw. \tag{1.73}$$

This gives the entry for $a_n = a$ in the table above.

1.3.2 The Random Packing

We wish to consider the properties of a dense random packing containing many spheres. We assume that the spheres occupy a large volume. The spheres are all identical in that they are the same size and have the same elastic moduli. They are large enough that we need not consider interaction forces such as capillary forces, Van der Waals forces and electrostatic interactions, which would become important for particles of diameter less than 200 μm (Troadec and Dodds [82], page 141).

In the undeformed configuration, the centre of a typical sphere, the nth say, will have position vector $\mathbf{X}^{(n)}$, relative to some given origin. This sphere will be in point contact with several of its neighbours. The boundary of the medium is subjected to a displacement $\mathbf{u}$ that is consistent with a uniform compressive strain e_{ij}, in order to reach the initial deformed configuration. Thus, the components of displacement have the form

$$u_i = e_{ij}x_j \tag{1.74}$$

where e_{ij} are the components of a symmetric constant tensor relative to some chosen axes. Although the medium is not continuous, we take e_{ij} to represent the average strain within the medium.

Under this deformation, the centre of the nth sphere say, will be displaced by an amount $\mathbf{u}^{(n)}$. Initially in contact with the nth we consider a second sphere, let this be the n'th. This also will undergo a displacement, $\mathbf{u}^{(n')}$, from its original position, $\mathbf{X}^{(n')}$. We neglect sphere rotations for now, but in a later section of this chapter, will look at the work carried out by Slade [76] to include these effects. Rotations are in fact significant in one of the initial configurations considered in Walton [86].

The position vector of the initial contact point is

$$\frac{1}{2}(\mathbf{X}^{(n)} + \mathbf{X}^{(n')}) \tag{1.75}$$

and from the symmetry of the problem, this will undergo a displacement

$$\frac{1}{2}(\mathbf{u}^{(n)} + \mathbf{u}^{(n')}). \tag{1.76}$$

Now the displacements of the sphere centres, relative to this point, for the nth and

n'th spheres are respectively

$$\frac{1}{2}(\mathbf{u}^{(n)} - \mathbf{u}^{(n')}) \quad \text{and} \quad \frac{1}{2}(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}). \tag{1.77}$$

The initial applied strain compresses the spheres together and small contact areas arise where there was originally a point contact. We wish to calculate the average stress within the medium and hence need to consider the force acting across each of these contact areas.

Each sphere, as we have already mentioned, is in contact with several of its neighbours and we need to consider the effect of the displacements and forces of one contact on the other contact areas. The usual way to deal with contact problems is to assume that the contact area is small in relation to the size of the body, as in the Hertz theory. As previously discussed, this enables the body to be approximated by an elastic half-space. Walton [84], when considering a purely normal compression acting on a regular packing, actually determined the displacements everywhere on the surface of the sphere. He showed that the displacements in the neighbourhood of the contact area are what would be expected under the Hertzian assumption. He also showed that for any physically interesting situations, the surface displacements are negligible apart from in the neighbourhood of the contact. Even though these results were only for a purely normal compression acting on the medium, it might be expected that this would also be the case for a general oblique compression. Thus to a good approximation, we assume that the contact areas can each be treated in isolation from one another.

For the contact we are considering, that is the one between the nth and n'th spheres, we wish to find the resultant stresses across the contact area when the sphere centres have been displaced by $\mp \frac{1}{2}(\mathbf{u}^{(\mathbf{n})} - \mathbf{u}^{(\mathbf{n}')})$ relative to the initial contact point. Initially, we again assume that the spheres are infinitely rough, the results for perfectly smooth spheres are given later. In section 1.2.2, we used the subscripts u and l to correspond to the half-spaces $z < 0$ and $z > 0$ respectively. We now take the lower sphere to be the nth and the upper to be the n'th. Introducing the unit vector, $\mathbf{I}^{(nn')}$, along the line of centres of the two spheres we have

$$\mathbf{I}^{(nn')} = \frac{\mathbf{X}^{(n)} - \mathbf{X}^{(n')}}{2R}. \tag{1.78}$$

To apply the results we have already found, we must split the displacement of the centre of each sphere into its normal and tangential components. Let the normal component of the relative displacement for the upper sphere be w_0, then this is given by

$$w_0 = \frac{1}{2}(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}. \tag{1.79}$$

As this is in the direction of $\mathbf{I}^{(nn')}$, the remainder of the relative displacement corresponds to the tangential part. Let this be $\mathbf{s}_0$, then we have

$$\mathbf{s}_0 = \frac{1}{2}(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}) - \frac{1}{2}\left((\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}\right)\mathbf{I}^{(nn')}. \tag{1.80}$$

The total force acting on the nth sphere, due to its contact with the n'th, can now be found using equations (1.59):

$$\begin{aligned} \mathbf{F}^{(nn')} &= \frac{4R^{1/2}w_0^{3/2}}{3\pi B}\mathbf{I}^{(nn')} + \frac{8(Rw_0)^{1/2}}{3\pi(2B+C)}\left\{\frac{1}{2}(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}) - w_0\mathbf{I}^{(nn')}\right\} \\ &= \frac{(2R)^{1/2}}{3\pi B(2B+C)}\{2B[(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{1/2}(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}) \\ &\qquad + C[(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{3/2}\mathbf{I}^{(nn')}\}. \end{aligned} \tag{1.81}$$

To determine this force we must make some kind of assumption about the relative displacement $(\mathbf{u}^{(n')} - \mathbf{u}^{(n)})$. Walton [86] follows the work of Digby [28] and Batchelor and O'Brien [1] in which the displacements of the sphere centres are assumed consistent with the applied uniform field. (In fact, Batchelor and O'Brien [1] deal with the problem of thermal and electrical conduction in a medium containing a large number of spherical inclusions). Thus we have

$$u_i^{(n)} = e_{ij}X_j^{(n)}, \tag{1.82}$$

which is often referred to as the uniform strain approximation. This is clearly consistent with equation (1.74) and although it will not be exact for every sphere, it will hold on average and so is a reasonable first approximation to make.

Now inserting equation (1.82) into equation (1.81) and using the definition of $\mathbf{I}^{(nn')}$ we have

$$F_i^{(nn')} = -\frac{4R^2}{3\pi B(2B+C)}\{2B(-e_{pq}I_p^{(nn')}I_q^{(nn')})^{1/2}e_{ij}I_j^{(nn')} - C(-e_{pq}I_p^{(nn')}I_q^{(nn')})^{3/2}I_i^{(nn')}\}. \tag{1.83}$$

This holds true for any general strain provided we ignore any rotation effects.

In order to calculate the effective elastic moduli of the medium we must determine the relationship between the average stress within the medium and the average strain, or equivalently, the uniform applied strain field e_{ij}. If V is the total volume occupied by the medium, that is the volume of both the spheres and the pore space, then the average stress $< \sigma_{ij} >$, over this volume, is given by

$$< \sigma_{ij} > \equiv \frac{1}{V}\int_{spheres} \sigma_{ij} dV = \frac{1}{V}\sum_n \int_{V_n} \sigma_{ij}^{(n)} dV \tag{1.84}$$

where V_n is the volume of the nth sphere, $\sigma_{ij}^{(n)}$ are the components of the Cauchy stress within this sphere and summation is over all the spheres, within the volume of the medium, V.

In particular, for the nth sphere, the integral on the right hand side of the previous equation can be re-written as an integral over the surface of that sphere. Thus,

$$\int_{V_n} \sigma_{ij} dV = \frac{1}{2}\int_{S_n} (x'_i t_j^{(n)} + x'_j t_i^{(n)}) dS \tag{1.85}$$

where the components $x'_i = x_i - X_i^{(n)}$ refer to the position vector of a material point of the sphere relative to its centre and $t_i^{(n)}$, the components of the traction across the surface of the sphere, S_n. The traction $t_i^{(n)}$ will be zero across the surface, except over the areas where the nth sphere is in contact with its neighbours. As seen in a previous section, this contact area is small in relation to the size of the sphere and thus for the contact between the nth and the n'th spheres, x'_i can be approximated as $\frac{1}{2}(X_i^{(n')} - X_i^{(n)})$. This is the position vector of the centre of the contact area, relative to the centre of the nth sphere and the integral of the traction on the contact area then reduces to $\mathbf{F}^{(nn')}$. Hence equation (1.85) becomes

$$\int_{V_n} \sigma_{ij} dV = \frac{1}{2}\sum_{n'}\left\{\frac{1}{2}\left(X_i^{(n')} - X_i^{(n)}\right)F_j^{(nn')} + \frac{1}{2}\left(X_j^{(n')} - X_j^{(n)}\right)F_i^{(nn')}\right\}, \tag{1.86}$$

the summation in this case taken over all spheres, n', in contact with the nth.

Our original expression for the total stress, equation (1.84), can thus be rewritten as

$$< \sigma_{ij} >= -\frac{R}{V} \sum \{ I_i^{(nn')} F_j^{(nn')} + I_j^{(nn')} F_i^{(nn')} \} \tag{1.87}$$

in which the summation this time is taken over all contacts, between all the spheres in the packing. The operator $< . >$ represents average over the total volume, V. The factor 1/2, does not appear in this equation as each contact occurs twice in the summation over both n and n'. We have already seen the expression for $\mathbf{F}^{(nn')}$ in equation (1.83) and this can be substituted into equation (1.87). Similar expressions appear in the work of Christoffersen *et al.* [18] and Cambou [13].

We have assumed that the packing is isotropic and that the contact points are uniformally distributed over the surface of each sphere. Since the volume is large and contains many spheres, the summation that arises from equation (1.87) can be written in terms of averages to yield:

$$\begin{aligned} < \sigma_{ij} > &= \frac{\phi\eta}{\pi^2 B(2B+C)} \{ B \langle (-e_{pq} I_p I_q)^{1/2} (e_{ik} I_k I_j + e_{jk} I_k I_i) \rangle \\ &\qquad - C \langle (-e_{pq} I_p I_q)^{3/2} I_i I_j \rangle \}. \end{aligned} \tag{1.88}$$

Here we have introduced η, the average number of contacts per sphere, that is the average coordination number and ϕ, which is the volume concentration of the spheres, defined by

$$\phi = \frac{4\pi R^3 N}{3V} \tag{1.89}$$

where R is again the radius of each sphere and N is the total number of spheres within the packing. The averaging operator, $< . >$ has different meanings, depending upon its position. On the left hand side it still represents average over the volume, but on the right hand side it represents average over all contacts within the packing.

Since our packing is dense then the porosity, γ, which is the ratio of the volume of the voids between the grains to the total volume of the packing, is between 0.36 and 0.38, Troadec and Dodds [82]. If instead, we were to consider a loose packing, this would be between 0.39 and 0.42. In fact, our particular calculations include the solid packing fraction, ϕ which is related to the porosity by $\phi = 1 - \gamma$ and hence we are looking at a value for ϕ of between 0.62 and 0.64, in our applications.

Equation (1.88), gives us the relationship we require between the average stress in the medium and average strain, which includes the effects of volume concentration and coordination number. These are properties of the packing and are assumed known. Scott [74] and Bernal and Mason [6] discuss the measurement of these quantities and statistical properties of random packings in general. There are several ways in which to determine the coordination number experimentally, for example,

- Acetic acid poured into a packing of lead spheres and then the liquid drained, the marks left on each sphere by lead acetate are counted, Smith *et al.* [78]. Careful examination allows real contacts to be distinguished from close neighbours. A similar experiment involves use of any kind of sphere and fast drying paint, Bernal and Mason [6].
- A sphere packing is impregnated with paraffin and the position of each sphere is then determined with precision as the packing is dismantled sphere by sphere, Bernal [5], Scott [75] and Mason and Clark [54].
- Bernal [4] used the method of compressing plastic balls together and counting the number of plane faces formed.

More recently, these quantities have been determined by numerical simulation.

Walton [86], only considers two specific cases of the application of an initial strain field, e_{ij}, as the expressions that arise in a general situation become very complicated. The two cases he considers are those of an initial hydrostatic strain and an initial uniaxial strain, although all the methods employed hold for any initial configuration.

Turning first then to the case of an initial hydrostatic strain, the applied strain field may be written as

$$e_{ij} = e\delta_{ij} \tag{1.90}$$

where e is a constant and thus upon substitution of this into equation (1.83) we find that the force acting on the nth sphere due to its contact with the n'th, reduces to the simple form

$$\mathbf{F}^{(nn')} = \frac{4R^2(-e)^{3/2}}{3\pi B}\mathbf{I}^{(nn')}. \tag{1.91}$$

Now, from equation (1.88), we find the average stress within the packing for this particular compression:

$$< \sigma_{ij} >= -\frac{\phi\eta(-e)^{3/2}}{\pi^2 B}\langle I_i I_j\rangle. \tag{1.92}$$

However, as

$$\langle I_i I_j\rangle = \frac{1}{3}\delta_{ij} \tag{1.93}$$

then

$$< \sigma_{ij} >= -p\delta_{ij} \tag{1.94}$$

where p is given by

$$p = \frac{\phi\eta(-e)^{3/2}}{3\pi^2 B}. \tag{1.95}$$

Secondly, we consider the case of uniaxial compression in the z-direction, then the strain field is given by

$$e_{ij} = e_3\delta_{i3}\delta_{j3} \tag{1.96}$$

where $e_3 < 0$ for compression. The resulting stress is then of the form

$$(< \sigma_{ij} >) = diag(< \sigma_1 >, < \sigma_1 >, < \sigma_3 >) \tag{1.97}$$

with

$$< \sigma_1 >= -\frac{\phi\eta C(-e_3)^{3/2}}{\pi^2 B(2B+C)}\langle |I_3|^3 I_1^2\rangle \tag{1.98}$$

and

$$< \sigma_3 >= -\frac{\phi\eta(-e_3)^{3/2}}{\pi^2 B(2B+C)}\{2B\langle |I_3| I_3^2\rangle + C\langle |I_3| I_3^4\rangle\}. \tag{1.99}$$

We require the value of the average terms and these are given in Walton [86] as:

$$\begin{aligned} < |I_3|^3 I_1^2 > &= \frac{1}{24} \\ < |I_3| I_3^2 > &= \frac{1}{4} \\ < |I_3| I_3^4 > &= \frac{1}{6} \end{aligned} \tag{1.100}$$

and so

$$< \sigma_1 >= -\frac{\phi n C(-e_3)^{3/2}}{24\pi^2 B(2B+C)} \tag{1.101}$$

and

$$< \sigma_3 >= -\frac{\phi n(3B+C)(-e_3)^{3/2}}{6\pi^2 B(2B+C)}. \tag{1.102}$$

These are the results in the case of infinitely rough spheres, if we now consider the case when they are perfectly smooth we observe that there will be no tangential forces acting across the contact area. By repeating all of the calculations above, but using equation (1.66) this time, we find the general average stress is given by

$$< \sigma_{ij} >= -\frac{\phi\eta^{(n)}}{\pi^2 B}\langle(-e_{pq}I_p^{(nn')}I_q^{(nn')})^{3/2}I_i^{(nn')}I_j^{(nn')}\rangle. \tag{1.103}$$

So, for an initial hydrostatic compression, the stress is the same as in the case of infinitely rough spheres. However, in the case of an initial uniaxial compression, this time we have

$$< \sigma_1 >= -\frac{\phi\eta^{(n)}(-e)^{3/2}}{24\pi^2 B} \tag{1.104}$$

and

$$< \sigma_3 >= -\frac{\phi\eta^{(n)}(-e)^{3/2}}{6\pi^2 B}. \tag{1.105}$$

1.3.3 The Effective Moduli

To calculate the effective moduli, we further subject the medium to an incremental deformation. That is, after the initial deformation, in the same way we now impose

$$\delta u_i = \delta e_{ij} x_j \tag{1.106}$$

on the boundary, where $\delta\mathbf{u}$ is consistent with a uniform strain δe_{ij}. Now, using the same methods as in the previous section, we find that the incremental force is given by

$$\begin{aligned}\delta\mathbf{F}^{(nn')} &= \frac{(2R)^{1/2}[(\mathbf{u}^{(n')}-\mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{1/2}}{2\pi B(2B+C)}\{2B(\delta\mathbf{u}^{(n')}-\delta\mathbf{u}^{(n)}) \\ &\quad +C[(\delta\mathbf{u}^{(n')}-\delta\mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]\mathbf{I}^{(nn')}\}.\end{aligned} \tag{1.107}$$

As before, we assume that the centre of the nth sphere will undergo a displacement

$$\delta u_i^{(n)} = \delta e_{ij} X_j^{(n)} \tag{1.108}$$

and then the average incremental stress is obtained in the same way as equation (1.88) and is given by:

$$\begin{aligned} < \delta\sigma_{ij} > &= \frac{3\phi\eta}{2\pi^2 B(2B+C)}\{B < (-e_{pq}I_pI_q)^{1/2}(\delta e_{ik}I_kI_j \\ &+\delta e_{jk}I_kI_i) > +C < (-e_pqI_pI_q)^{1/2}I_kI_lI_iI_j > \delta e_{kl}\}. \end{aligned} \quad (1.109)$$

This expression relates the average incremental stress to the average incremental strain. Since the effective moduli C^*_{ijkl} are defined by

$$< \delta\sigma_{ij} >= C^*_{ijkl} < \delta e_{kl} > \quad (1.110)$$

then the general expression for the moduli is given by

$$\begin{aligned} C^*_{ijkl} &= \frac{3\phi\eta}{2\pi^2 B(2B+C)}\{B < (-e_{pq}I_pI_q)^{1/2}I_jI_k > \delta_{il} \\ &+B < (-e_{pq}I_pI_q)^{1/2}I_iI_k > \delta_{jl} + B < (-e_{pq}I_pI_q)^{1/2}I_jI_l > \delta_{ik} \quad (1.111) \\ &+B < (-e_{pq}I_pI_q)^{1/2}I_iI_l > \delta_{jk} + 2C < (-e_{pq}I_pI_q)^{1/2}I_iI_jI_kI_l >\}. \end{aligned}$$

We want C^*_{ijkl} to possess symmetries in:

$$i)\ i \leftrightarrow j \quad ii)\ k \leftrightarrow l \quad iii)\ (ij) \leftrightarrow (kl) \text{ or equivalently } i \leftrightarrow k \text{ and } j \leftrightarrow l, \quad (1.112)$$

and our expression clearly satisfies these. The elastic moduli are seen to depend on the initial strain and in general our medium is now no longer isotropic. We again consider our two cases of hydrostatic and uniaxial compression so that equation (1.111) simplifies. First, with an initial hydrostatic strain $e_{ij} = e\delta_{ij}$, equation (1.111) reduces to

$$\begin{aligned} C^*_{ijkl} &= \frac{3\phi\eta(-e)^{1/2}}{4\pi^2 B(2B+C)}\{B < I_jI_k > \delta_{il} + B < I_iI_k > \delta_{jl} + B < I_jI_l > \delta_{ik} \\ &\qquad +B < I_iI_l > \delta_{jk} + 2C < I_iI_jI_kI_l >\}. \end{aligned} \quad (1.113)$$

However, as before we have

$$< I_iI_j >= \frac{1}{3}\delta_{ij} \quad (1.114)$$

and now also

$$< I_iI_jI_kI_l >= \frac{1}{15}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \quad (1.115)$$

Thus,

$$C^*_{ijkl} = \lambda^* \delta_{ij}\delta_{kl} + \mu^*(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{1.116}$$

where

$$\lambda^* = \frac{\phi\eta C(-e)^{1/2}}{10\pi^2 B(2B+C)} \tag{1.117}$$

and

$$\mu^* = \frac{\phi\eta(5B+C)(-e)^{1/2}}{10\pi^2 B(2B+C)}. \tag{1.118}$$

In this case the material is statistically isotropic.

Secondly, in the case of uniaxial compression, $e_{ij} = e_3\delta_{i3}\delta_{j3}$ and the moduli reduce to

$$\begin{aligned} C^*_{ijkl} &= \frac{3\phi n(-e_3)^{1/2}}{4\pi^2 B(2B+C)}\{B < |I_3|I_jI_k > \delta_{il} + B < |I_3|I_iI_k > \delta_{jl} \\ &\quad +B < |I_3|I_jI_l > \delta_{ik} + B < |I_3|I_iI_l > \delta_{jk} + 2C < |I_3|I_iI_jI_kI_l >\}. \end{aligned} \tag{1.119}$$

This time the material is statistically transversely isotropic and calculating the averages of the components of $\mathbf{I}^{(nn')}$ we see that the effective moduli are as follows:

$$\begin{aligned} C^*_{11} &= C^*_{1111} = 3(\alpha + 2\beta), \\ C^*_{12} &= C^*_{1122} = \alpha - 2\beta, \\ C^*_{13} &= C^*_{1133} = C^*_{2233} = 2C^*_{12}, \\ C^*_{33} &= C^*_{3333} = 8(\alpha + \beta), \\ C^*_{44} &= C^*_{1313} = 2\alpha + 5\beta, \end{aligned} \tag{1.120}$$

with

$$\alpha = \frac{\phi\eta(-e_3)^{1/2}}{32\pi^2 B}, \tag{1.121}$$

and

$$\beta = \frac{\phi\eta(-e_3)^{1/2}}{32\pi^3(2B+C)}. \tag{1.122}$$

We note that the modulus C^*_{44} is different to the incorrect one given by equation (4.14) of Walton [86]. These are the results when the spheres have an infinite coefficient of friction.

Looking again also at the case when the spheres are perfectly smooth, in the case of an initial hydrostatic compression the moduli are equal and are given by

$$\lambda^* = \mu^* = \frac{\phi\eta(-e)^{1/2}}{10\pi^2 B} \tag{1.123}$$

and in the case of an initial uniaxial compression,

$$C_{11}^* = 3\alpha,\ C_{12}^* = \alpha,\ C_{13}^* = C_{44}^* = 2\alpha, C_{33}^* = 8\alpha \tag{1.124}$$

where α is again as given above in equation (1.121).

These results are extended in the work of Slade and Walton [77], where a finite, non-zero value of the coefficient of friction was considered for the particular case of an initial uniaxial compression, followed by an incremental uniaxial compression. The general form for the incremental strain when there is finite friction was also considered by Slade [76].

The above results for the moduli have been determined using the same methods as Walton [86], however Slade [76], has shown the need for consideration of the individual sphere rotations. When we do include rotations, we find that in fact the only moduli we have incorrectly calculated is C_{44}^* for the uniaxial case. The next section summarises Slade's work on this problem.

1.3.4 Sphere Rotations Within Random Packings

Walton [86] assumed that although the individual spheres in the packing might rotate, these rotations would be negligible. As we shall see, this is valid, provided particular symmetries exist in the way the packing is initially deformed. In a further paper, Walton [87] did consider the effects of rotations when studying the problem of wave propagation through a random packing of spheres. Including rotations into the calculations, the centre of the nth sphere now undergoes a displacement $(\mathbf{u}^{(n)} - \omega^{(n)} \wedge R\mathbf{I}^{(nn')})$ and the n'th in contact with the nth, a displacement $(\mathbf{u}^{(n')} - \omega^{(n')} \wedge R\mathbf{I}^{(n'n)})$. Thus, the modified equation for the initial force acting on the nth sphere due to its contact with the n'th is given by equation (2.8) of Walton's paper as:

$$\begin{aligned}\mathbf{F}^{(nn')} &= \frac{(2R)^{1/2}}{3\pi B(2B+C)}\{2B[(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{1/2}(\mathbf{u}^{(n')} - \mathbf{u}^{(n)} \\ &\quad +(\omega^{(n')} + \omega^{(n)}) \wedge R\mathbf{I}^{(nn')}) + C[(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{3/2}\mathbf{I}^{(nn')}\},\end{aligned}$$

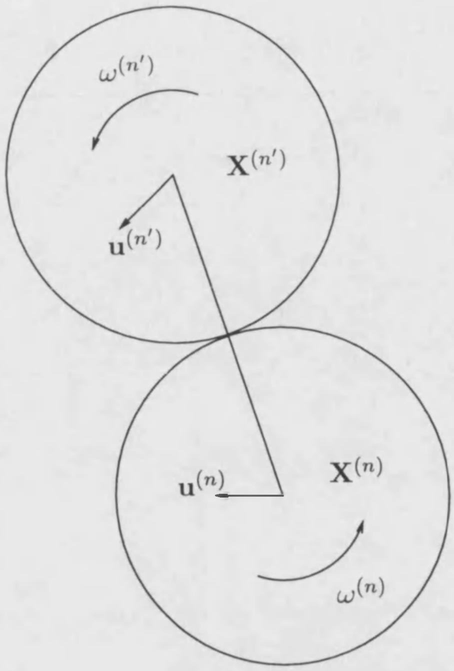

Figure 1-4: *Initial Deformation of Two Spheres Including Rotations*

(1.125)

where R is again the radius of the spheres and $\mathbf{l}^{(nn')}$, the unit vector along the line of centres between the nth and n'th spheres. The displacement of the centres of the nth and n'th spheres after the initial compression are $\mathbf{u}^{(n)}$ and $\mathbf{u}^{(n')}$, respectively and B and C are as before. The quantities $\omega^{(n)}$ and $\omega^{(n')}$ are the individual rotations of spheres n and n' respectively. Figure 1-4 shows the initial deformation of the nth sphere in contact with the n'th. We use the same notation as before so that the centre of the nth sphere is initially at $\mathbf{X}^{(n)}$.

Any packing we consider will be in equilibrium and so each individual sphere must also be in equilibrium. Hence we require that the sum of the forces and moments acting on a sphere must be zero. Thus, for the nth sphere, say,

$$\sum_{n'} \mathbf{F}^{(nn')} = \mathbf{0} \tag{1.126}$$

and

$$\sum_{n'} \mathbf{l}^{(nn')} \wedge \mathbf{F}^{(nn')} = \mathbf{0}. \tag{1.127}$$

These, along with equation (1.125) provide enough conditions, in theory, to calculate $\mathbf{u}^{(n)}$ and $\omega^{(n)}$ for any sphere, n. In Walton [86], it was assumed that a good approximation was to take the rotation terms, $\omega^{(n)}$, as zero and the displacements, $\mathbf{u}^{(n)}$, as given by the uniform strain approximation.

Now, from equation (1.127) it follows that

$$\sum_{n'} I_i^{(nn')} F_j^{(nn')} = \sum_{n'} I_j^{(nn')} F_i^{(nn')}$$

and so

$$\sum_{contacts} I_i^{(nn')} F_j^{(nn')} = \sum_{contacts} I_j^{(nn')} F_i^{(nn')}.$$

Writing this in terms of the averaging operator, $< . >$, we have

$$< I_i F_j >=< I_j F_i >, \tag{1.128}$$

which if not satisfied with the exclusion of rotations from equation (1.125) would suggest that rotations need to be included. We then assume that the displacements $\mathbf{u}^{(n)}$ are still given by the uniform strain approximation but that the rotations, $\omega^{(n)}$ are the same for each sphere throughout the packing. An expression for $\omega^{(n)}$ can then be determined using equation (1.128).

Similarly, from the other equilibrium condition, equation (1.126), we have

$$< F_i >= 0, \tag{1.129}$$

which should be automatically satisfied, but can be checked for any particular case of initial compression as we shall see below.

The Initial Deformed State

Slade [76], considers the same two cases of initial confining strain as did Walton [86], that is he considers first a hydrostatic strain and secondly a uniaxial one. From equation (3.6) of Walton [86] we have already seen that the general expression for the force without rotations is given by equation (1.83), that is

$$F_i^{(nn')} = -\frac{4R^2}{3\pi B(2B+C)}\{2B(-e_{pq}I_p^{(nn')}I_q^{(nn')})^{1/2}e_{ij}I_j^{(nn')} - C(-e_{pq}I_p^{(nn')}I_q^{(nn')})^{3/2}I_i^{(nn')}\}. \tag{1.130}$$

This then gives

$$< I_iF_j > \; = \; -\frac{4R^2}{3\pi B(2B+C)}\left\{2B\langle(-e_{pq}I_pI_q)^{1/2}e_{jk}I_kI_i\rangle - C\langle(-e_{pq}I_pI_q)^{3/2}I_iI_j\rangle\right\} \tag{1.131}$$

so that now we can consider the specific strain cases mentioned.

In the case of a hydrostatic compression we have

$$e_{ij} = e\delta_{ij} \tag{1.132}$$

with $e < 0$ corresponding to compression. In this case, equation (1.131) becomes

$$< I_iF_j >= \frac{4R^2(-e)^{3/2}}{3\pi B} < I_iI_j > \tag{1.133}$$

and it is clearly symmetric in i and j. Hence, the average stress due to an initial hydrostatic compression can be calculated as

$$< \sigma_{ij} >= -\frac{\phi\eta(-e)^{3/2}}{\pi^2 B} < I_iI_j > \tag{1.134}$$

which is precisely that calculated by Walton [86] and seen in Section 1.3.2. By a geometrical argument, the same conclusion could have been reached. Under a hydrostatic compression, the forces acting on an individual sphere to rotate it clockwise would be exactly balanced by those acting to turn it anticlockwise.

Considering also the second case, an initial uniaxial compression along the z-axis we have

$$e_{ij} = e_3\delta_{i3}\delta_{j3} \tag{1.135}$$

in which $e_3 < 0$. Again calculating $< I_iF_j >$ from equation (1.131), we find

$$< I_iF_j >= -\frac{4R^2(-e_3)^{3/2}}{3\pi B(2B+C)}\{2B < |I_3|I_3I_i > \delta_{j3} + C < |I_3|^3 I_iI_j >\}. \tag{1.136}$$

The second term, with coefficient C, is seen to be symmetric in i and j, however we need to explicitly calculate the other term to decide if it too is symmetric. Slade [76] evaluates this as zero when $i = 1$ or $i = 2$ and $1/4$ when $i = 3$. This enables us to rewrite the term as:

$$< |I_3| I_3 I_i > \delta_{j3} =< |I_3| I_3^2 > \delta_{i3}\delta_{j3}, \tag{1.137}$$

which is clearly symmetric in i and j. We find that the average stress resulting from an initial uniaxial strain remains unchanged from that which is given in equation (3.24) of Walton [86].

We have seen that in both the application of an initial hydrostatic compression and that of a uniaxial compression, the average rotation of the spheres was zero and did not have any effect on the expression for the average stress. This is not the case when we consider the incremental stage of the problem, rotations are required to ensure equilibrium of moments.

Application of an Additional Incremental Strain

Relative to the contact point with position vector $(\mathbf{X}^{(n)} + \mathbf{X}^{(n')})/2$, the incremental displacement of the centre of the n'th sphere will be

$$\frac{1}{2}(\delta\mathbf{u}^{(n')} - \delta\mathbf{u}^{(n)}) + \frac{1}{2}(\delta\omega^{(n')} + \delta\omega^{(n)}) \wedge R\mathbf{I}^{(nn')}. \tag{1.138}$$

This displacement can be split into its normal and tangential parts in the same way as considered by Walton [86] and as discussed in Section 1.3.2. The normal component of the relative displacement of the upper sphere δw_0, is found to be

$$\delta w_0 = \frac{1}{2}(\delta\mathbf{u}^{(n')} - \delta\mathbf{u}^{(n)}).\mathbf{I}^{(nn')} \tag{1.139}$$

The shear component, which is the remainder of the relative displacement, is then given as follows:

$$\delta\mathrm{s}_0 = \frac{1}{2}(\delta\mathbf{u}^{(n')} - \delta\mathbf{u}^{(n)}) + \frac{1}{2}(\delta\omega^{(n')} + \delta\omega^{(n)}) \wedge R\mathbf{I}^{(nn')} - \delta w_0\mathbf{I}^{(nn')}. \tag{1.140}$$

The incremental force vector can be constructed from the incremental normal and tangential forces found from these displacements. This will be the incremental form of equation (1.125):

$$\delta \mathbf{F}^{(nn')} = \frac{(2R)^{1/2}[(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{1/2}}{2\pi B(2B+C)}\{2B(\delta \mathbf{u}^{(n')} - \delta \mathbf{u}^{(n)} + (\delta\omega^{(n')} + \delta\omega^{(n)}) \wedge R\mathbf{I}^{(nn')}) + C[(\delta \mathbf{u}^{(n')} - \delta \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{3/2}\mathbf{I}^{(nn')}\}. \tag{1.141}$$

We now make the same assumption as before, that the displacements of the centre of each sphere is consistent with the applied uniform field. Thus,

$$u_i^{(n)} = e_{ij}X_j^{(n)} \tag{1.142}$$

and

$$\delta u_i^{(n)} = \delta e_{ij}X_j^{(n)} \tag{1.143}$$

and a similar assumption will be made about the rotations. Since we assume that the strain field is uniform throughout the packing then we also assume that the spheres all rotate by the same amount, that is

$$\delta\omega^{(n)} = \delta\omega^{(n')} = \delta\omega. \tag{1.144}$$

Again, as with the displacements, each sphere will not rotate by exactly the amount given, but it will be true on average. Now, using the definition of the unit normal vector, equation (1.78), we have from equation (1.141) the component form of the incremental force given as:

$$\delta F_i^{(nn')} = -\frac{2R^2(-e_{pq}I_pI_q)^{1/2}}{\pi B(2B+C)}\{C\delta e_{kl}I_kI_lI_i + 2B\delta e_{il}I_l - 2B\epsilon_{ikl}\delta\omega_k I_l\}. \tag{1.145}$$

The superscripts (nn') of the vector components I_i, have been omitted for brevity, ϵ_{ikl} is the third order alternating tensor.

Equilibrium Conditions

If the nth sphere is to be in equilibrium we require the sum of all the incremental forces acting on it to be zero and the sum of the moments of those forces to also be zero. Hence, we have

$$\sum_{n'} \mathbf{I}^{(nn')} \wedge \delta\mathbf{F}^{(nn')} = \mathbf{0} \tag{1.146}$$

$$\sum_{n'} \delta \mathbf{F}^{(nn')} = \mathbf{0}. \tag{1.147}$$

Substituting from equation (1.145) into equation (1.146), after disregarding one term as it will be zero, the condition for equilibrium of moments reduces to:

$$\sum_{n'} (-e_{pq} I_p I_q)^{1/2} (\delta_{ik} - I_i I_k) \delta\omega_k = \sum_{n'} \epsilon_{irk} (-e_{pq} I_p I_q)^{1/2} I_r I_l \delta e_{kl}. \tag{1.148}$$

Summation is taken over all spheres n' in contact with the nth sphere and by also summing over all spheres n, provided we have a dense enough packing the summation may be written in terms of averages yielding,

$$\langle (-e_{pq} I_p I_q)^{1/2} (\delta_{ik} - I_i I_k) \rangle \delta\omega_k = \epsilon_{irk} \langle (-e_{pq} I_p I_q)^{1/2} I_r I_l \rangle \delta e_{kl} \tag{1.149}$$

from which the incremental rotation vector $\delta\omega$ may be determined in terms of the incremental strain δe_{ij} which is known. Slade [76] calculates the components of this as

$$\delta\omega_1 = -\frac{1}{3}\delta e_{23}, \;\; \delta\omega_2 = \frac{1}{3}\delta e_{13}, \;\; \delta\omega_3 = 0. \tag{1.150}$$

We also have the condition for equilibrium of the incremental forces, equation (1.147), which becomes

$$\langle (-e_{pq} I_p I_q)^{1/2} \{ C I_k I_l I_i + B \delta_{ik} I_l \} \delta e_{kl} \rangle = 2B \epsilon_{ikl} \langle (-e_{pq} I_p I_q)^{1/2} I_l \delta\omega_k \rangle. \tag{1.151}$$

Any initial compression would in fact satisfy this condition since we are averaging over odd quantities.

The Incremental Stress

Equation (1.109), gives the general form of the incremental stress and having determined the rotation vector $\delta\omega$ from equation (1.149), we can substitute the expression for the incremental force from equation (1.145) to find this incremental stress. We obtain,

$$\begin{aligned} < \delta\sigma_{ij} > \;\; &= \;\; \frac{3\phi\eta}{2\pi^2 B(2B+C)} \Big\{ C \langle (-e_{pq} I_p I_q)^{1/2} I_i I_j I_k I_l \delta e_{kl} \rangle \\ &\quad + 2B \langle (-e_{pq} I_p I_q)^{1/2} I_l I_i \delta e_{jl} \rangle - 2B \epsilon_{ikl} \langle (-e_{pq} I_p I_q)^{1/2} I_i I_l \delta\omega_k \rangle \Big\} \end{aligned} \tag{1.152}$$

from which the effective moduli can be found in the same way as before.

Slade [76], considers first the case of an initial hydrostatic strain for which we have $e_{ij} = e\delta_{ij}$. The incremental stress is symmetric before inclusion of the rotation term above. Thus the calculations are unaffected by rotations and so the moduli are as found by Walton [86] and seen in Section 1.3.2.

However, in the case of an initial uniaxial strain we have $e_{ij} = e_3\delta_{i3}\delta_{j3}$ and the incremental stress is found to be

$$\begin{aligned} < \delta\sigma_{ij} > &= \frac{3\eta\phi(-e)^{1/2}}{2\pi^2 B(2B+C)} \{(B < |I_3|I_i I_l > \delta_{jk} > +B < |I_3|I_i I_k > \\ &\quad +C < |I_3|I_i I_j I_k I_l >) < \delta e_{kl} > -2B\epsilon_{jpq} < |I_3|I_q I_i > \delta\omega_p\} . \end{aligned} \tag{1.153}$$

The New Effective Elastic Moduli

As we have found the incremental rotation vector, we can proceed to find the incremental stress from which the revised effective moduli will be calculated. If we compare equation (1.153), the expression for the incremental stress including rotations with that found by Walton [86] without rotations, we see that equation (1.153) contains an extra term, $\epsilon_{jpq} < I_i I_q |I_3| > \delta\omega_p$. Slade [76] concludes that this is zero for $i = j$. Since we require the indices j, p and q to be distinct, then in particular $j \neq q$. If $< I_i I_q |I_3| >$ is to be non-zero then we must have $i = q$ which combined with the previous condition gives us $i \neq j$ for $\epsilon_{jpq} < I_i I_q |I_3| > \delta\omega_p$ non-zero. Hence, in fact only one of the five independent elastic moduli is affected by the inclusion of rotations.

The elastic moduli are defined by the relationship

$$< \delta\sigma_{ij} >= C^*_{ijkl} < \delta e_{kl} > \tag{1.154}$$

and taking $i = j = 1$ in equation (1.153) gives the three moduli

$$\begin{aligned} C^*_{1111} &= \frac{3\phi\eta(-e_3)^{1/2}(4B+C)}{32\pi^2 B(2B+C)}, \\ C^*_{1122} &= \frac{\phi\eta C(-e_3)^{1/2}}{32\pi^2 B(2B+C)}, \\ C^*_{1133} &= \frac{\phi\eta(-e_3)^{1/2} C}{16\pi^2 B(2B+C)}. \end{aligned} \tag{1.155}$$

Similarly, if $i = j = 3$, then

$$C^*_{3333} = \frac{\phi\eta(-e_3)^{1/2}(3B + C)}{4\pi^2 B(2B + C)}. \tag{1.156}$$

These four moduli, are identical to those calculated by Walton [86], however if we take $i = 1$ and $j = 3$ then the rotation term is non-zero and in this case the required moduli is found by Slade [76] to be

$$C^*_{1313} = \frac{\phi\eta(-e_3)^{1/2}(4B + C)}{16\pi^2 B(2B + C)}. \tag{1.157}$$

Re-writing all of these moduli in terms of α and β as before, we see that we have the five independent effective elastic moduli needed to describe a transversely isotropic medium:

$$\begin{aligned} C^*_{11} &= 3(\alpha + 2\beta), \\ C^*_{12} &= (\alpha - 2\beta), \\ C^*_{13} &= 2(\alpha - 2\beta), \\ C^*_{33} &= 8(\alpha + \beta), \\ C^*_{44} &= 2(\alpha + 2\beta). \end{aligned} \tag{1.158}$$

The quantities α and β are defined as before by

$$\alpha = \frac{\phi\eta(-e_3)^{1/2}}{32\pi^2 B}, \quad \beta = \frac{\phi\eta(-e_3)^{1/2}}{32\pi^2(2B + C)}. \tag{1.159}$$

Using a physical argument, these results are exactly what we would expect, that is only the modulus $C^*_{44} = C^*_{1313}$ is affected by the rotations that occur within the packing. Since we are considering an initial uniaxial strain, the contact areas created upon application of this strain will not all be of equal radius as they would in the case of an initial hydrostatic strain. Those that are created between two spheres whose line of centres is in the same direction as the strain, i.e. in the x_3-direction, will be the largest. These contact areas themselves lie in the x_1x_2-plane. Conversely, those contacts that lie in the same direction as the strain will be smallest.

First consider the moduli C^*_{11}, C^*_{12} and C^*_{13} that arise from the relationship between the stress component σ_{11} and the strain components e_{11}, e_{22} and e_{33} respectively. The stress component σ_{11} corresponds to a force acting in the x_1-direction. If the contact distribution is uniform, as we have assumed, then this force will act on identical sized contacts on opposite sides of a sphere. Therefore we would expect the effects of rotations due to this force to 'cancel' each other out. Hence the corresponding moduli are also not affected. Similarly for C^*_{33}, which is found from the relationship between σ_{33} and e_{33}. However, the modulus C^*_{44} is determined from the relationship between σ_{13} and e_{13}. The stress component σ_{13} represents a shear acting in the x_1 and x_3 directions which will result in the same force acting on different sized contact areas. This will lead to imbalance, the moments will not now cancel and rotation effects will appear within the expression for this modulus.

1.4 Alternatives to the Uniform Strain Approximation

All the calculations discussed thus far to find the effective elastic moduli have been based upon the uniform strain approximation. Several authors have considered alternative approaches in effective medium theory. Here we mention briefly some of this work, although we will not use the ideas in this thesis. In particular, we mention a method that could be described as a 'uniform stress approximation'.

In their work, Emeriault and Cambou [33], suggest three methods of deriving a macroscopic elastic model from a microscopic contact law (Hertz-Mindlin). They consider a random packing of spheres, both isotropic and anisotropic, although we are purely interested in their results for isotropic media. They consider the global variables, σ_{ij} and e_{ij}, these are the stress and strain tensors respectively, in the same notation we have used. The local variables are the contact forces, F_i and the relative displacement of contact points between particles, U_i. The first order approximations of these are $\overline{F}_i$ and $\overline{U}_i$. The average diameter of the spheres is $2R$.

The local variables involved in the homogenisation technique are only quoted in Emeriault and Cambou [33], the actual discussion of them can be found elsewhere, Cambou *et al.* [14]. These variables are:

$$\text{StaticVariable}: \qquad \mathbf{f(I)} = \frac{2(1+d)\pi NR}{3V} P(\mathbf{I})\overline{\mathbf{F}}(\mathbf{I}) \tag{1.160}$$

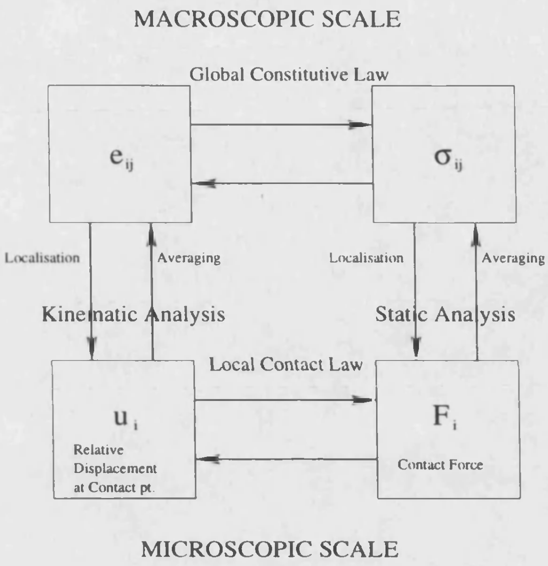

Figure 1-5: *Different Localisation and Averaging Operators*

$$\text{KinematicVariable}: \qquad \mathbf{u}(\mathbf{I}) \; = \frac{3}{2(1+d)\pi R}\overline{U}(\mathbf{I}) \tag{1.161}$$

where $P(\mathbf{I})$ is the contact distribution function and is equal to $1/4\pi$ in the case of an isotropic medium and d is the dimension of the space, so in our case $d = 3$.

All three methods discussed by Emeriault and Cambou [33], relate to finding the operators to describe various paths around the boxes in figure 1 of Emeriault and Cambou [33], shown here in figure 1-5. Different hypotheses are used to consider the localisation and averaging processes in this diagram. The three approaches as described by Emeriault and Cambou [33] are as follows:

1. Voigt type process: $\mathbf{e} \xrightarrow{L_1^k} \mathbf{u}(\mathbf{I})$ and $\mathbf{f}(\mathbf{I}) \xrightarrow{A_1^s} \sigma$.
2. Static localisation process: $\sigma \xrightarrow{L_2^s} \mathbf{f}(\mathbf{I})$ and $\mathbf{u} \xrightarrow{A_2^k} \epsilon$.
3. Second Kinematic localisation process: $\mathbf{e} \xrightarrow{L_3^k} \mathbf{u}(\mathbf{I})$ and $\mathbf{f}(\mathbf{I}) \xrightarrow{A_3^s} \sigma$.

In each of these methods, A stands for an averaging operator, L for a localisation, s for static analysis and k for kinematic analysis and the numbers represent the process that uses the operator. Both the first and third approaches follow the same path around the diagram as the uniform strain approximation. In fact the first is identical, yielding the expressions we have already considered for the effective moduli. It is described by Emeriault and Cambou [33] as a Voigt type process, as the localisation operator relating the strain to the displacement is equivalent to the classical one used in Voigt's homogenisation in continuum mechanics.

The second and third approaches yield new expressions for the effective moduli. The second approach traverses the box diagram in the opposite direction to the uniform strain approximation and could be described as a uniform stress approximation. Using the representation theorem, Spencer [79], the operator L_2^s, is found, exactly, to be

$$\mathbf{f}(\mathbf{I}) = \mu\sigma\mathbf{I} + \frac{1-\mu}{2}(5\mathbf{I}\sigma\mathbf{I} - tr\sigma)\mathbf{I}. \tag{1.162}$$

A simple linear contact model is assumed to connect the contact force to the displacement in the following way:

$$\mathbf{F} = K_n U_n \mathbf{I} + K_t \mathbf{U}_t \tag{1.163}$$

where U_n is the magnitude of the displacement in the normal direction, $\mathbf{U}_t$ is the displacement in the tangential direction and K_n and K_t respectively denote the normal and tangential stiffness. The averaging process, A_2^k is described by

$$\mathbf{e} = \int_{Unit\ Sphere} \left[\mu\mathbf{u} \wedge \mathbf{I} + \frac{1-\mu}{2}[5\mathbf{I} \wedge \mathbf{I} - \delta]\mathbf{u}.\mathbf{I}\right] d\Theta, \tag{1.164}$$

where $d\Theta$ is the solid angle for each contact orientation $\mathbf{I}$. The parameter μ is used to define the local operator, its value influences the orientation of the contact forces. From these hypotheses, the shear modulus is found to be

$$\mu^* = \frac{5\phi\eta(-e)^{1/2}}{B(25 - 30\mu) + 3\mu^2(5B + C)} \tag{1.165}$$

and the bulk modulus is found to be the same using all three approaches, hence

$$\kappa^* = \frac{\phi\eta(-e)^{1/2}}{6\pi^2 B}. \tag{1.166}$$

Emeriault and Cambou [33] compared the theoretical values given by these results with some experimental work and found that a value of approximately $\mu^* = 0$ gives good correlation. However, a value $\mu = 0.7$ was found from numerical simulations to give a better description of the contact force distribution. Apart from the fact that this unknown variable is included, we decided not to consider a further use of this model because of the unrealistic linear relationship between the force and displacement, equation (1.163).

Returning to the third process discussed in this paper, an application of the representation theorem is again used, this time to find that the localisation operator, L_3^k is

$$\mathbf{u}(\mathbf{I}) = \frac{3}{4\pi}\left\{\left[1 + b\left(\frac{3\mu}{5} - 1\right)\right]\mathbf{e}\mathbf{I} + b\left[\mathbf{I}\mathbf{e}\mathbf{I} - \frac{\mu}{5}tre\right]\mathbf{I}\right\}. \tag{1.167}$$

The averaging operator, A_3^s is the same as that we use in the uniform strain approximation to connect the average stress to the force:

$$\sigma = \frac{3}{4\pi}\int_{Unit\ Sphere} \mathbf{f}\wedge\mathbf{I}d\Omega. \tag{1.168}$$

The local operator contains another unknown parameter b, when $b = 0$ we return to the first approach again. Emeriault and Cambou [33] connect this parameter b to the local rotation of particles and to the possible creation and loss of contacts in the medium and so the first approach eliminates any possible rotations. We have already mentioned the consequence of this in the previous section. The shear modulus in this third case is calculated as

$$\mu^* = \frac{\phi\eta(-e)^{1/2}(5B + C - 3Bb + \frac{3}{5}(5B + C)b\mu)}{5\pi^2 B(2B + C)} \tag{1.169}$$

and the bulk modulus is as in the other two approaches. The shear modulus again contains the unknown parameters μ and b and for this reason we have not considered any further application of this method.

Several other authors have done some similar work, including Mülhaus and Oka [56] and Chang *et al.* [16]. Chang *et al.* [16] calculate the effective moduli by considering a kinematic and static hypotheses similar to the work of Emeriault and Cambou [33] discussed above. The expression for the effective bulk modulus is identical in all cases, it is only the effective shear modulus where there is some difference. Chang *et al.* [16] claim that the kinematic hypothesis, for example the one by Walton [86] discussed in detail in previous sections, provides an upper bound solution for a relationship to estimate the particle movement. It is also claimed that the static hypothesis provides a lower estimate solution. Chang *et al.* [16] compare the results obtained from both of these methods with the range of behaviour of isotropic and anisotropic packing structures. However, both this paper and that of Mülhaus and Oka [56] again assume that the relationship between the force on the contact area and the displacement is linear. Hence we do not consider them to be as realistic as the model by Walton [86].

Chapter 2

Effective Elastic Moduli of Granular Media Subjected to a General Biaxial Strain

2.1 Introduction

As we have mentioned in section 1.3.2, the work of Walton [86] employs a method that could be used to consider any initial deformed configuration, although specific results are only given for the two cases that correspond to an initial hydrostatic compression and a uniaxial compression. The work in this chapter is an extension of the method to a third case and we calculate the effective elastic moduli for an initial biaxial compression. Like Walton [86], for simplicity, we assume that the spheres are either infinitely rough or perfectly smooth.

The work of Schwartz *et al.* [73] has already extended Walton's work by considering a perturbation of the strain for an initial hydrostatic compression. The paper looks at two types of model for predicting induced velocity anisotropy in rocks. It is the first of these methods that is concerned with a combined initial hydrostatic compression and uniaxial loading. That is, the initial strain has the form:

$$e_{ij} = e\delta_{ij} + \Delta e_3 \delta_{i3}\delta_{j3}. \tag{2.1}$$

where $\Delta e_3 \ll e$. The models he uses for this were developed by himself, Schwartz [71], Schwartz *et al.* [72] and that of Walton [86], discussed in the previous chapter.

Firstly, we look at this case of applied strain and recalculate the moduli since Schwartz *et al.* [73] did not consider the effect of the inclusion of rotations on the moduli. Using the results in section 1.3.4 found by Slade [76], we calculate the effective moduli both including and excluding the effects of rotations. It turns out that in this case again only the modulus C^*_{1313} is affected by rotations.

Later in the chapter the case of a general biaxial compression is considered. Assuming a spatial coordinate system given by x_1, x_2, and x_3 our aim is to calculate the effective elastic moduli when we have an initial strain of the form:

$$e_{ij} = e_1(\delta_{i1}\delta_{j1} + \delta_{i2}\delta_{j2}) + e_3\delta_{i3}\delta_{j3}. \tag{2.2}$$

As in Schwartz *et al.* [73], relative to this state the material is transversely isotropic with five independent moduli C^*_{1111}, C^*_{1133}, C^*_{3333}, C^*_{1313} and C^*_{1212}. By considering the symmetry of the expression found for the average incremental stress we show that the sphere rotations do not affect the moduli C^*_{1111}, C^*_{1133}, C^*_{3333}, and C^*_{1212}, however they do affect C^*_{1313}. Therefore C^*_{1313} will be calculated both including and excluding rotations. Schwartz *et al.* [73] use these moduli to calculate the ratio of the speeds of propagation of the P and S elastic sound waves in rock. That is, three independent $(V_p/V_s)^2$ ratios: C^*_{3333}/C^*_{1313}, C^*_{1111}/C^*_{1212} and C^*_{1111}/C^*_{1313}. The first corresponds to propagation along the pressure axis, that is the x_3-axis, the second to propagation in the transverse direction with the shear wave polarised in the transverse plane and the third to transverse propagation with shear polarization in the axial direction.

Domenico [30] found that for systems whose elastic properties are isotropic under the application of a hydrostatic stress, the V_P/V_S ratio, is often independent of the applied pressure. That is, the ratio of the velocity of the P and S waves may be independent of the applied pressure, even though the P and S wave velocities themselves may vary with this pressure. However, this is not the case when the applied strain is uniaxial as the systems exhibit transversely isotropic behaviour and the three V_P/V_S ratios do depend on the applied strain. (See Nur and Simmons [61], Murphy [59], Zamora and Poirier [95] and Yin and Nur [94]).

We are considering a system of this second type and plot graphs of the three V_P/V_S

ratios against the third component of stress for two values of Poisson's ratio, 1/2 and 1/4. We compare them with figure 1 of Schwartz *et al.* [73], which plots the experimental results of Murphy [59] and calculated V_P/V_S ratios.

All the analysis in Walton [86] which leads to the general results that were summarised in Section 1.3.2, are initially completed for the general case. Thus we can quote some of the results without need for reworking of the calculations. We start by restricting ourselves to the case of infinitely rough spheres, the results for perfectly smooth spheres are given later.

The spheres are assumed to be elastically identical, all of the same radius and consisting of material that is homogenous and isotropic. To see the effects of sphere rotations which are non-zero we initially exclude them from the calculations. Equation (1.83) gives the contact force, without rotations, as

$$\begin{aligned} F_i^{(nn')} &= -\frac{4R^2}{3\pi B(2B+C)} \Big\{ 2B(-e_{pq}I_p^{(nn')}I_q^{(nn')})^{1/2} e_{ik} I_k^{(nn')} \\ &\qquad -C(-e_{pq}I_p^{(nn')}I_q^{(nn')})^{3/2} I_i^{(nn')} \Big\}, \end{aligned} \tag{2.3}$$

from which the average stress can be calculated. The average stress, at the end of the initial compression, is as given in equation (1.87), that is

$$\langle \sigma_{ij} \rangle = -\frac{R}{V} \sum_{\text{contacts}} \left\{ I_i^{(nn')} F_j^{(nn')} + I_j^{(nn')} F_i^{(nn')} \right\}. \tag{2.4}$$

Since the volume is large and contains many spheres, the summation over all contacts within the packing volume V, can be replaced by the averaging operator $< . >$, as seen previously, thus

$$< \sigma_{ij} >= -\frac{R\eta N}{2V} \left\{ \langle I_i F_j \rangle + \langle I_j F_i \rangle \right\}. \tag{2.5}$$

Using equation (2.3) we find the average quantity $< I_i F_j >$, and then equation (1.88) is given as:

$$\begin{aligned} < \sigma_{ij} > &= \frac{\phi\eta}{\pi^2 B(2B+C)} \{ B\langle (-e_{pq}I_pI_q)^{1/2}(e_{ik}I_kI_j + e_{jk}I_kI_i) \rangle \\ &\qquad -C\langle (-e_{pq}I_pI_q)^{3/2} I_iI_j \rangle \}. \end{aligned} \tag{2.6}$$

To calculate the effective moduli we further subject the medium to an incremental deformation. That is, after the initial deformation we impose an incremental displacement

$$\delta u_i = \delta e_{ij} x_j \tag{2.7}$$

on the boundary, where δu_i is consistent with a uniform strain δe_{ij}. We calculate the incremental force using equation (1.107) and the average incremental stress is then obtained in the same way as equation (2.6), that is we have equation (1.109)

$$\begin{aligned} < \delta\sigma_{ij} > &= \frac{3\phi\eta}{2\pi^2 B(2B+C)}\{B < (-e_{pq}I_pI_q)^{1/2}(\delta e_{ik}I_kI_j \\ &+\delta e_{jk}I_kI_i) > +C < (-e_{pq}I_pI_q)^{1/2}I_kI_lI_iI_j > \delta e_{kl}\}. \end{aligned} \tag{2.8}$$

This expression relates the average incremental stress to the average incremental strain and since the effective moduli C^*_{ijkl} are defined by

$$< \delta\sigma_{ij} >= C^*_{ijkl}\delta e_{kl} \tag{2.9}$$

then the general expression for the moduli is given by equation (1.111) as

$$\begin{aligned} C^*_{ijkl} &= \frac{3\phi n}{2\pi^2 B(2B+C)}\{B < (-e_{pq}I_pI_q)^{1/2}I_jI_k > \delta_{il} \\ &+B < (-e_{pq}I_pI_q)^{1/2}I_iI_k > \delta_{jl} + B < (-e_{pq}I_pI_q)^{1/2}I_jI_l > \delta_{ik} \\ &+B < (-e_{pq}I_pI_q)^{1/2}I_iI_l > \delta_{jk} + 2C < (-e_{pq}I_pI_q)^{1/2}I_iI_jI_kI_l >\}. \end{aligned} \tag{2.10}$$

since this possesses all the appropriate symmetries. We will include rotations into this analysis later in the chapter.

2.2 Perturbation of an Initial Hydrostatic Compression

2.2.1 The Initial State

For a hydrostatic strain we have

$$e_{ij} = e\delta_{ij}, \tag{2.11}$$

and as already seen, equation (2.1), we wish to calculate the effective elastic moduli when this strain is perturbed in one direction. Thus, we consider a strain of the form:

$$e_{ij} = e\delta_{ij} + \Delta e_3\delta_{i3}\delta_{j3} \tag{2.12}$$

where $\Delta e_3 \ll e$. We assume, as did Walton [86], that the displacement of the centre of each sphere is consistent with the applied uniform field, so that

$$u_{ij}^{(n)} = e_{ij} X_j^{(n)}. \tag{2.13}$$

We substitute this displacement into the general force expression which then allows us to calculate the average stress. For now, we still ignore any effects that sphere rotations may introduce and use equation (2.6) to find the average stress. This gives:

$$\begin{aligned} <\sigma_{ij}> \;=\; & \frac{\phi n}{\pi^2 B(2B+C)}\{B < (-(e+I_3^2\Delta e_3))^{1/2}(eI_iI_j \\ & +\Delta e_3\delta_{i3}I_3I_j + eI_jI_i + \Delta e_3\delta_{j3}I_3I_i) > \\ & -C < (-(e+I_3^2\Delta e_3))^{3/2}I_iI_j >\}. \end{aligned} \tag{2.14}$$

But, working to first order only in $\Delta e_3/e$,

$$(e+I_3^2\Delta e_3)^{1/2} \simeq e^{1/2}(1+\frac{1}{2}I_3^2\frac{\Delta e_3}{e}) \tag{2.15}$$

since $\Delta e_3 \ll e$, and similarly,

$$(e+I_3^2\Delta e_3)^{3/2} \simeq e^{3/2}(1+\frac{3}{2}I_3^2\frac{\Delta e_3}{e}). \tag{2.16}$$

We also have that

$$\begin{aligned} < I_iI_j > \;&=\; \frac{1}{3}\delta_{ij} \\ < I_iI_jI_kI_l > \;&=\; \frac{1}{15}(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}), \end{aligned} \tag{2.17}$$

so then the average stress $<\sigma_{ij}>$ reduces to

$$\begin{aligned} <\sigma_{ij}> \;=\; & \frac{\phi\eta}{\pi^2 B(2B+C)}\{-(2B+C)(-e)^{3/2}\frac{\delta_{ij}}{3}+\frac{2}{3}B(-e)^{1/2}\Delta e_3\delta_{i3}\delta_{j3} \\ & +\frac{1}{15}(B-\frac{3}{2}C)(-e)^{1/2}\Delta e_3(\delta_{ij}+2\delta_{i3}\delta_{j3})\}. \end{aligned} \tag{2.18}$$

Hence we see that

$$(<\sigma_{ij}>) = \text{diag}\,(<\sigma_{11}>, <\sigma_{11}>, <\sigma_{33}>), \tag{2.19}$$

where

$$\begin{aligned}
<\sigma_{11}> &= \frac{\phi\eta}{\pi^2 B(2B+C)}\{-\frac{1}{3}(2B+C)(-e)^{3/2}+\frac{1}{15}(B+\frac{3}{2}C)(-e)^{1/2}\Delta e_3\}, \\
<\sigma_{33}> &= \frac{\phi\eta}{\pi^2 B(2B+C)}\{-\frac{1}{3}(2B+C)(-e)^{3/2}+\frac{1}{30}(16B+9C)(-e)^{1/2}\Delta e_3\}.
\end{aligned} \tag{2.20}$$

These results apply to the case of infinitely rough spheres. Now considering the case when all the spheres are perfectly smooth there will be no shear force across the contact area. Repeating the analysis, then equation (2.6) for the average stress becomes:

$$<\sigma_{ij}>=-\frac{\phi\eta}{\pi^2 B}\langle(-e_{pq}I_pI_q)^{3/2}I_iI_j\rangle \tag{2.21}$$

in the general case. In the case of a perturbed hydrostatic strain as we are considering, equations (2.20) reduce to

$$\begin{aligned}
<\sigma_{11}> &= -\frac{\phi\eta(-e)^{3/2}}{3\pi^2 B}\{1+\frac{3}{10}(-e)^{-1/2}\Delta e_3\}, \\
<\sigma_{33}> &= -\frac{\phi\eta(-e)^{3/2}}{3\pi^2 B}\{1+\frac{9}{10}(-e)^{-1/2}\Delta e_3\}.
\end{aligned} \tag{2.22}$$

2.2.2 The Incremental Problem

We apply a further incremental displacement to the boundary

$$\delta u_i = \delta e_{ij}x_j \tag{2.23}$$

again assuming that the displacement of each sphere centre is consistent with this applied uniform field. This enables us to calculate the incremental force acting across the contact area between the nth and n'th spheres, from which we find the incremental stress.

From equation (2.9) and again using the approximation in equation (2.15), the elastic moduli are given by:

$$\begin{aligned}
C^*_{ijkl} &= \frac{3\phi\eta}{4\pi^2 B(2B+C)}\Big\{B(-e)^{1/2}\{<I_jI_k>\delta_{il}+<I_iI_k>\delta_{jl}+<I_jI_l>\delta_{ik} \\
&\quad +<I_iI_l>\delta_{jk}\}+2C(-e)^{1/2}<I_iI_jI_kI_l>
\end{aligned}$$

$$+\frac{B}{2}(-e)^{-1/2}\Delta e_3\{< I_3^2 I_j I_k > \delta_{il} + < I_3^2 I_i I_k > \delta_{jl} + < I_3^2 I_j I_l > \delta_{ik}$$
$$+ < I_3^2 I_i I_l > \delta_{jk}\} + C\Delta e_3(-e)^{-1/2} < I_3^2 I_i I_j I_k I_l >\Big\}. \qquad (2.24)$$

Using equations (2.17) and the further equality

$$\begin{aligned}\langle I_3^2 I_i I_j I_k I_l\rangle &= \frac{1}{105}\{\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} + 2(\delta_{ij}\delta_{k3}\delta_{l3} \\ &\quad +\delta_{ik}\delta_{j3}\delta_{l3} + \delta_{il}\delta_{j3}\delta_{k3} + \delta_{i3}(\delta_{jk}\delta_{l3} + \delta_{jl}\delta_{k3} + \delta_{kl}\delta_{j3}))\}, \end{aligned} \qquad (2.25)$$

and if we define

$$\alpha = \frac{\phi\eta}{140\pi^2 B}, \quad \beta = \frac{\phi\eta}{140\pi^2(2B+C)}, \quad \gamma = 14\alpha, \quad \delta = 14\beta, \qquad (2.26)$$

then we now have enough information to calculate the moduli and they can be written concisely as

$$\begin{aligned} C_{11}^* &\equiv C_{1111}^* = (-e)^{1/2}(3\gamma + 4\delta) - \Delta e_3(-e)^{-1/2}(3\alpha + 8\beta), \\ C_{12}^* &\equiv C_{1122}^* = (-e)^{1/2}(\gamma - 2\delta) - \Delta e_3(-e)^{-1/2}(\alpha - 2\beta), \\ C_{13}^* &\equiv C_{1133}^* = C_{2233}^* = (-e)^{1/2}(\gamma - 2\delta) - \Delta e_3(-e)^{-1/2}(3\alpha - 6\beta), \\ C_{33}^* &\equiv C_{3333}^* = (-e)^{1/2}(3\gamma + 4\delta) - \Delta e_3(-e)^{-1/2}(15\alpha + 12\beta), \\ C_{44}^* &\equiv C_{1313}^* = (-e)^{1/2}(3\gamma - \delta) - \Delta e_3(-e)^{-1/2}(3\alpha + 8\beta). \end{aligned} \qquad (2.27)$$

For completeness, we calculate the remaining non-zero modulus defined by

$$C_{66}^* \equiv C_{1212}^* = (-e)^{1/2}(\gamma + 3\delta) + \Delta e_3(-e)^{-1/2}(\alpha + 5\beta). \qquad (2.28)$$

For a transversely isotropic medium such as the one we are considering, Mal and Singh [52], show that only the five moduli given in equation (2.27), are independent and this sixth modulus can be expressed in terms of the other elastic constants as

$$C_{66}^* = \frac{1}{2}(C_{11}^* - C_{12}^*). \qquad (2.29)$$

A quick calculation shows that this relationship is confirmed and we have just the five independent elastic moduli in equation (2.27).

We again use the notation

$$C^*_{1111} = C^*_{11}, \qquad C^*_{1122} = C^*_{12}, \qquad C^*_{1133} = C^*_{13},$$
$$C^*_{3333} = C^*_{33}, \quad C^*_{1313} = C^*_{2323} = C^*_{55} = C^*_{44} \quad C^*_{1212} = C^*_{66}. \tag{2.30}$$

This is the notation used in Schwartz *et al.* [73] and makes later comparison easier.

The results in equation (2.27) only apply for the case when the spheres are infinitely rough. When we now consider the spheres as perfectly smooth we find that the moduli are given by

$$\begin{aligned}
C^*_{11} &= 3\gamma(-e)^{1/2} + 3\alpha\Delta e_3(-e)^{-1/2},\\
C^*_{12} &= \gamma(-e)^{1/2} + \alpha\Delta e_3(-e)^{-1/2},\\
C^*_{13} &= \gamma(-e)^{1/2} + 3\alpha\Delta e_3(-e)^{-1/2},\\
C^*_{33} &= 3\gamma(-e)^{1/2} + 15\alpha\Delta e_3(-e)^{-1/2},\\
C^*_{44} &= \gamma(-e)^{1/2} + 3\alpha\Delta e_3(-e)^{-1/2},\\
C^*_{66} &= 3\gamma(-e)^{1/2} + \alpha\Delta e_3(-e)^{-1/2},
\end{aligned} \tag{2.31}$$

where α and γ are as defined in equation (2.26). Again, there are just the five independent moduli, C^*_{66} can be expressed as a combination of C^*_{11} and C^*_{12} (see equation (2.29)).

2.2.3 Inclusion of the Effects of Rotations

We now recalculate the elastic moduli for the initial strain given in equation (2.12), but this time include the effects of rotations of the individual spheres. For the initial problem, we need an expression for the term $< I_i F_j >$, which is found to be:

$$\begin{aligned}
< I_i F_j > \; &= \; \frac{-4R^2}{3\pi B(2B+C)}\{2B(-e)^{1/2}(< (e + \frac{1}{2}I_3^2\Delta e_3)I_iI_j > + \Delta e_3\delta_{j3} < I_3 I_i >)\\
&\qquad -C(-e)^{1/2} < (e + \Delta e_3 I_3^2 + \frac{1}{2}\Delta e_3 I_3^2)I_iI_j >\}.
\end{aligned} \tag{2.32}$$

Clearly the first and last terms of this expression are symmetric in i and j. If we consider $\delta_{j3} < I_3 I_i >$, this is non-zero if and only if $i = j = 3$ and so this term is also symmetric in i and j. Thus $< I_i F_j >$ is symmetric in i and j and hence so is $< \sigma_{ij} >$, and individual sphere rotations do not have any effect on this part of the problem.

Thus, the average stress of the material after the initial compression is indeed given by equations (2.19) and (2.20), namely,

$$(<\sigma_{ij}>) = \text{diag}\,(<\sigma_{11}>, <\sigma_{11}>, <\sigma_{33}>), \tag{2.33}$$

and

$$\begin{aligned} <\sigma_{11}> &= \frac{\phi\eta}{\pi^2 B(2B+C)}\{-\frac{1}{3}(2B+C)(-e)^{3/2} + \frac{1}{15}(B+\frac{3}{2}C)(-e)^{1/2}\Delta e_3\} \\ <\sigma_{33}> &= \frac{\phi\eta}{\pi^2 B(2B+C)}\{-\frac{1}{3}(2B+C)(-e)^{3/2} + \frac{1}{30}(16B+9C)(-e)^{1/2}\Delta e_3\}. \end{aligned} \tag{2.34}$$

When we have perfectly smooth spheres the average stress is again as given in equation (2.22).

Results from the second chapter of Slade [76] are required to continue with the second part of the problem, the incremental stage. These are the conditions for equilibrium, which allow us to calculate the components of rotation and the general expression for the average incremental stress. These give the two equations:

$$<(-e_{pq}I_pI_q)^{1/2}\{CI_kI_lI_i + B\delta_{ik}I_l\}\delta e_{kl}> -2B\epsilon_{ikl} <(-e_{pq}I_pI_q)^{1/2}I_l\delta\omega_k> = 0 \tag{2.35}$$

and

$$<(-e_{pq}I_pI_q)^{1/2}(\delta_{ik} - I_iI_k)> \delta\omega_k = \epsilon_{irk} <(-e_{pq}I_pI_q)^{1/2}I_rI_l> \delta e_{kl}, \tag{2.36}$$

the first of which corresponds to equilibrium of the incremental forces, equation (1.151) and the second to equilibrium of moments equation (1.149). The incremental stress now contains an extra term, due to rotations, which was absent from our last calculation of the moduli. This stress is given by equation (1.109) as:

$$\begin{aligned} <\delta\sigma_{ij}> = \frac{3\eta\phi}{2\pi^2 B(2B+C)}\{&C <(-e_{pq}I_pI_q)^{1/2}I_iI_jI_kI_l\delta e_{kl}> \\ &+2B <(-e_{pq}I_pI_q)^{1/2}I_lI_i\delta e_{jl}> -2B\epsilon_{jkl} <(-e_{pq}I_pI_q)^{1/2}I_iI_l\delta\omega_k>\}. \end{aligned} \tag{2.37}$$

We first check that equation (2.35) holds, that is that the forces acting are in equilibrium. Substituting for the strain field (2.12), into equation (2.35), gives

$$
\begin{aligned}
&< (-e)^{1/2}\left(1+\frac{1}{2}I_3^2\frac{\Delta e_3}{e}\right)\{CI_kI_lI_i + B\delta_{ik}I_l\} > \delta e_{kl} \\
&-2B\epsilon_{ikl} < (-e)^{1/2}\left(1+\frac{1}{2}I_3^2\frac{\Delta e_3}{e}\right)I_l > \delta\omega_k \quad = \quad 0 \qquad (2.38)
\end{aligned}
$$

By the symmetry of the components of **I** on the interval over which they are averaged we have

$$
< I_kI_lI_i >=< I_3^2I_kI_lI_i >=< I_l >= 0 \qquad (2.39)
$$

and so clearly this equilibrium condition holds, irrespective of the components of rotation.

If we now take equation (2.36) and substitute for our particular strain field we can calculate the components of rotation,

$$
\begin{aligned}
&< (-e)^{1/2}\left(1+\frac{1}{2}I_3^2\frac{\Delta e_3}{e}\right)(\delta_{ik} - I_iI_k) > \delta\omega_k \\
&= \epsilon_{irk} < (-e)^{1/2}\left(1+\frac{1}{2}I_3^2\frac{\Delta e_3}{e}\right)I_rI_l > \delta e_{kl} \qquad (2.40)
\end{aligned}
$$

which yields

$$
\begin{aligned}
&< \delta_{ik} - I_iI_k + \frac{\delta_{ik}}{2}I_3^2\frac{\Delta e_3}{e} - \frac{1}{2}\frac{\Delta e_3}{e}I_3^2I_iI_k > \delta\omega_k \\
&= \epsilon_{irk} < I_rI_l + \frac{1}{2}\frac{\Delta e_3}{e}I_3^2I_rI_l > \delta e_{kl}. \qquad (2.41)
\end{aligned}
$$

Putting $i = 1$ in this last we find that

$$
\delta\omega_1 = -\frac{\Delta e_3}{2(5e+\Delta e_3)}\delta e_{23} \qquad (2.42)
$$

and similarly putting $i = 2$ and $i = 3$ respectively, we see that

$$
\delta\omega_2 = \frac{\Delta e_3}{2(5e+\Delta e_3)}\delta e_{13} \qquad (2.43)
$$

and

$$
\delta\omega_3 = 0. \qquad (2.44)
$$

We can now use these in equation (2.37) to find the components of the incremental stress. Putting $i = j = 1$ in (2.37) we can find the three moduli C_{11}^*, C_{12}^* and C_{13}^*. There are no effects due to the rotations for these three moduli and so using the same notation as before, the moduli are:

$$\begin{aligned}
C_{11}^* &= (-e)^{1/2}(3\gamma + 4\delta) + \Delta e_3(-e)^{-1/2}(3\alpha + 8\beta), \\
C_{12}^* &= (-e)^{1/2}(\gamma - 2\delta) + \Delta e_3(-e)^{-1/2}(\alpha - 2\beta), \\
C_{13}^* &= (-e)^{1/2}(\gamma - 2\delta) + \Delta e_3(-e)^{-1/2}(3\alpha - 6\beta).
\end{aligned} \tag{2.45}$$

Similarly, putting $i = j = 3$ we have no effect due to the rotations and thus

$$C_{33}^* = (-e)^{1/2}(3\gamma + 4\delta) + \Delta e_3(-e)^{-1/2}(15\alpha + 12\beta). \tag{2.46}$$

To find C_{44}^*, we calculate $< \sigma_{13} >$ which is given by

$$\begin{aligned}
< \sigma_{13} > \; = \; & \frac{3n\phi(-e)^{1/2}}{2\pi^2 B(2B + C)} \Big\{ [B(< I_l I_1 > + \frac{1}{2}\frac{\Delta e_3}{e} < I_3^2 I_l I_1 >)\delta_{3k} \\
& + B(< I_k I_1 > + \frac{1}{2}\frac{\Delta e_3}{e} < I_3^2 I_1 I_k >)\delta_{3l} \\
& + C(< I_1 I_3 I_k I_l > + \frac{1}{2}\frac{\Delta e_3}{e} < I_3^3 I_1 I_k I_l >)] < \delta e_{kl} > \\
& - 2B(\epsilon_{321}[< I_1^2 > + \frac{1}{2}\frac{\Delta e_3}{e} < I_3^2 I_1^2 >] < \delta\omega_2 > \\
& + \epsilon_{312}[< I_1 I_2 > + \frac{1}{2}\frac{\Delta e_3}{e} < I_3^2 I_1 I_2 >] < \delta\omega_1 >) \Big\}.
\end{aligned} \tag{2.47}$$

The first of the terms due to rotation effects is not eliminated in this case and we recalculate C_{44}^* as

$$C_{44}^* = (-e)^{1/2}(\gamma + 3\delta) + \Delta e_3(-e)^{-1/2}(3\alpha + 8\beta), \tag{2.48}$$

where α, β, γ and δ are as before.

In fact, this is the only modulus affected by considering rotations, C_{1212}^* is unaffected and so we again have our five independent moduli given by

$$\begin{aligned}
C_{11}^* &= (-e)^{1/2}(3\gamma + 4\delta) - \Delta e_3(-e)^{-1/2}(3\alpha + 8\beta), \\
C_{12}^* &= (-e)^{1/2}(\gamma - 2\delta) - \Delta e_3(-e)^{-1/2}(\alpha - 2\beta), \\
C_{13}^* &= (-e)^{1/2}(\gamma - 2\delta) - \Delta e_3(-e)^{-1/2}(3\alpha - 6\beta),
\end{aligned} \tag{2.49}$$

$$
\begin{aligned}
C^*_{33} &= (-e)^{1/2}(3\gamma + 4\delta) - \Delta e_3(-e)^{-1/2}(15\alpha + 12\beta), \\
C^*_{44} &= (-e)^{1/2}(\gamma + 3\delta) - \Delta e_3(-e)^{-1/2}(3\alpha + 8\beta).
\end{aligned}
$$

These are the moduli for infinitely rough spheres.

In the instance when the spheres are perfectly smooth, the moduli are

$$
\begin{aligned}
C^*_{11} &= 3\gamma(-e)^{1/2} + 3\alpha\Delta e_3(-e)^{-1/2}, \\
C^*_{12} &= \gamma(-e)^{1/2} + \alpha\Delta e_3(-e)^{-1/2} \\
C^*_{13} &= \gamma(-e)^{1/2} + 3\alpha\Delta e_3(-e)^{-1/2}, \\
C^*_{33} &= 3\gamma(-e)^{1/2} + 15\alpha\Delta e_3(-e)^{-1/2}, \\
C^*_{44} &= \gamma(-e)^{1/2} + 3\alpha\Delta e_3(-e)^{-1/2}.
\end{aligned} \tag{2.50}
$$

These are identical to those found in equations (2.31) since there is no tangential traction with perfectly smooth spheres and so there are no rotations to include in the calculations.

2.3 The Effective Elastic Moduli for an Initial General Biaxial Strain

We now extend the case considered in the previous section to that of a general biaxial strain. As already mentioned, we calculate an expression for the stress and the elastic moduli in the case of an initial strain of the form:

$$
\begin{aligned}
e_{ij} &= e_1(\delta_{i1}\delta_{j1} + \delta_{i2}\delta_{j2}) + e_3\delta_{i3}\delta_{j3} \\
&= e_1\delta_{ij} + (e_3 - e_1)\delta_{i3}\delta_{j3}.
\end{aligned} \tag{2.51}
$$

This is a generalisation of the strain in equation (2.12).

Assuming that the displacement of the sphere centres is consistent with the uniform strain field, as before, and from the subsequent general expression for the force derived by Walton [86], we find the force acting across the contact area on the nth sphere due to its contact with the n'th from equation (2.3) is:

$$\begin{aligned} F_i^{(nn')} &= \frac{4R^2(-e_1)^{3/2}}{3\pi B(2B+C)}\left\{2B\left[1+\frac{e_3-e_1}{e_1}I_3^2\right]^{1/2}\right. \\ &\quad \left. x(I_i+\frac{(e_3-e_1)}{e_1}\delta_{i3}I_3) - C\left[1+\frac{e_3-e_1}{e_1}I_3^2\right]^{3/2} I_i\right\}. \end{aligned} \tag{2.52}$$

2.3.1 Stress Components

The general expression for the average stress is given in equation (2.6),

$$\begin{aligned} \langle\sigma_{ij}\rangle &= \frac{\phi\eta}{\pi^2 B(2B+C)}\{B\langle(-e_{pq}I_pI_q)^{1/2}(e_{ik}I_kI_j+e_{jk}I_kI_i)\rangle \\ &\qquad -C\langle(-e_{pq}I_pI_q)^{3/2}I_iI_j\rangle\}. \end{aligned} \tag{2.53}$$

Substituting in the expression for the general biaxial strain as given in equation (2.51), we can calculate the stress. A typical average arising in the calculation is

$$\langle(-e_{pq}I_pI_q)^{1/2}I_3^2\rangle \equiv \frac{1}{4\pi}\int_0^{2\pi}d\phi\int_0^{\pi}(-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}\cos^2\theta\sin\theta d\theta. \tag{2.54}$$

This and other similar integrals that arise, may be evaluated using standard techniques (see Appendix A). We define

$$f_1(x) = \begin{cases} x^{1/2} + \frac{1}{(1-x)^{1/2}}\sin^{-1}(1-x)^{1/2} & \text{if } x<1 \\ 2 & \text{if } x=1 \\ x^{1/2} + \frac{1}{(x-1)^{1/2}}\sinh^{-1}(x-1)^{1/2} & \text{if } x>1 \end{cases} \tag{2.55}$$

$$f_2(x) = \begin{cases} \frac{x^{1/2}(1-2x)}{4(1-x)} + \frac{1}{4(1-x)^{3/2}}\sin^{-1}(1-x)^{1/2} & \text{if } x<1 \\ 2/3 & \text{if } x=1 \\ \frac{x^{1/2}(2x-1)}{4(x-1)} - \frac{1}{4(x-1)^{3/2}}\sinh^{-1}(x-1)^{1/2} & \text{if } x>1 \end{cases} \tag{2.56}$$

$$f_3(x) = \begin{cases} \frac{x^{1/2}(3-2x)}{4(1-x)} + \frac{(3-4x)}{4(1-x)^{3/2}}\sin^{-1}(1-x)^{1/2} & \text{if } x<1 \\ 4/3 & \text{if } x=1 \\ \frac{x^{1/2}(2x-3)}{4(x-1)} + \frac{(4x-3)}{4(x-1)^{3/2}}\sinh^{-1}(x-1)^{1/2} & \text{if } x>1 \end{cases} \tag{2.57}$$

Then, also using equation (2.51), we obtain a stress tensor that has purely diagonal non-zero entries, as was the case earlier in this chapter,

$$(\langle\sigma_{ij}\rangle) = \text{diag }(\langle\sigma_1\rangle, \langle\sigma_1\rangle, \langle\sigma_3\rangle) \tag{2.58}$$

where

$$\begin{aligned}
\langle\sigma_1\rangle &= -\frac{\phi\eta(-e_1)^{3/2}}{4\pi^2 B(2B+C)}\left\{(2B+\frac{3C}{4})f_1\left(\frac{e_3}{e_1}\right)-(2B+\frac{C}{2})f_2\left(\frac{e_3}{e_1}\right)+\frac{C}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\},\\
\langle\sigma_3\rangle &= -\frac{\phi\eta(-e_1)^{3/2}}{\pi^2 B(2B+C)}\left\{(\frac{Be_3}{e_1}+\frac{C}{4})f_2\left(\frac{e_3}{e_1}\right)+\frac{C}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\}.
\end{aligned} \tag{2.59}$$

So, in particular

$$-\frac{\pi^2 B(2B+C)}{\phi\eta C(-e_1)^{3/2}}\langle\sigma_3\rangle = (\frac{B}{C}\frac{e_3}{e_1}+\frac{1}{4})f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{6}\left(\frac{e_3}{e_1}\right)^{3/2}. \tag{2.60}$$

For the case where Poisson's ratio, $\nu = 1/4$, then $B/C = 3$ and so

$$k_1\langle\sigma_3\rangle = (\frac{3e_3}{e_1}+\frac{1}{4})f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{6}\left(\frac{e_3}{e_1}\right)^{3/2}, \tag{2.61}$$

where

$$k_1 = -\frac{\pi^2 B(2B+C)}{\phi\eta C(-e_1)^{3/2}} = -\frac{21\pi^2}{\phi\eta(-e_1)^{3/2}}. \tag{2.62}$$

Similarly, for $\nu = 1/2$, $B/C = 1$ and

$$k_2\langle\sigma_3\rangle = (\frac{e_3}{e_1}+\frac{1}{4})f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{6}\left(\frac{e_3}{e_1}\right)^{3/2}, \tag{2.63}$$

where

$$k_2 = -\frac{\pi^2 B(2B+C)}{\phi\eta C(-e_1)^{3/2}} = -\frac{3\pi^2}{\phi\eta(-e_1)^{3/2}}. \tag{2.64}$$

We will use this scaled version of $\langle\sigma_3\rangle$ later when we come to plot the graphs.

For comparison with Schwartz *et al.* [73], we only need consider these results, that is the results for the case when the spheres are infinitely rough. However for completeness, we also find the average stress when the spheres are perfectly smooth. This is calculated to be:

$$(\langle\sigma_{ij}\rangle) = \text{diag }(\langle\sigma_1\rangle,\langle\sigma_1\rangle,\langle\sigma_3\rangle) \tag{2.65}$$

where

$$\begin{aligned}
\langle\sigma_1\rangle &= -\frac{\phi\eta(-e_1)^{3/2}}{4\pi^2 B}\left\{\frac{3}{4}f_1\left(\frac{e_3}{e_1}\right)-\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\},\\
\langle\sigma_3\rangle &= -\frac{\phi\eta(-e_1)^{3/2}}{\pi^2 B(2B+C)}\left\{\frac{1}{4}f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\}.
\end{aligned} \tag{2.66}$$

2.3.2 The Effective Moduli Without Rotation Effects

To calculate the effective moduli we find the average incremental stress, equation (2.8). From this expression, which holds for any strain, we then have the following general expression for the moduli C^*_{ijkl}, equation (4.6) in Walton [86] and previously given in equation (2.10),

$$\begin{aligned} C^*_{ijkl} &= \frac{3\phi\eta}{2\pi^2 B(2B+C)}\{B\langle(-e_{pq}I_pI_q)^{1/2}I_jI_k\rangle\delta_{il} + B\langle(-e_{pq}I_pI_q)^{1/2}I_iI_k\rangle\delta_{jl} \\ &\quad + B\langle(-e_{pq}I_pI_q)^{1/2}I_jI_l\rangle\delta_{ik} + B\langle(-e_{pq}I_pI_q)^{1/2}I_iI_l\rangle\delta_{jk} \\ &\quad + 2C\langle(-e_{pq}I_pI_q)^{1/2}I_iI_jI_kI_l\rangle\}. \qquad (2.67) \end{aligned}$$

The integrals that arise are similar to those met in equation (2.54) and using the subscript mapping defined in equation (2.30), we find that

$$\begin{aligned} C^*_{11} &= \frac{3\phi\eta(-e_1)^{1/2}}{4\pi^2 B(2B+C)}\left\{Bf_3\left(\frac{e_3}{e_1}\right) + \frac{3}{8}C\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(\frac{1}{2} - \frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)} + f_3\left(\frac{e_3}{e_1}\right)\right]\right\}, \\ C^*_{12} &= \frac{3\phi\eta C(-e_1)^{1/2}}{32\pi^2 B(2B+C)}\left\{\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(\frac{1}{2} - \frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)} + f_3\left(\frac{e_3}{e_1}\right)\right\}, \\ C^*_{13} &= \frac{3\phi\eta C(-e_1)^{1/2}}{8\pi^2 B(2B+C)}\left\{\frac{-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(-\frac{1}{2} + \frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)}\right\}, \qquad (2.68) \\ C^*_{33} &= \frac{3\phi\eta(-e_1)^{1/2}}{4\pi^2 B(2B+C)}\left\{2Bf_2\left(\frac{e_3}{e_1}\right) + C\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} - \frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)}\right]\right\}, \\ C^*_{44} &= \frac{3\phi\eta(-e_1)^{1/2}}{8\pi^2 B(2B+C)}\left\{\frac{B}{2}f_3\left(\frac{e_3}{e_1}\right) + Bf_2\left(\frac{e_3}{e_1}\right) + C\left[\frac{-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(\frac{e_3}{e_1} - \frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)}\right]\right\}, \\ C^*_{66} &= \frac{3\phi\eta(-e_1)^{1/2}}{4\pi^2 B(2B+C)}\left\{\frac{B}{2}f_3\left(\frac{e_3}{e_1}\right) + \frac{C}{8}\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(-\frac{e_3}{e_1} + \frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)} + f_3\left(\frac{e_3}{e_1}\right)\right]\right\}. \end{aligned}$$

As the medium we consider is again transversely isotropic, these constants are related by $C^*_{12} = C^*_{11} - 2C^*_{66}$, leaving just five that are independent. These expressions were new at the time of derivation, however, shortly after, we discovered that they were simultaneously derived by Schwartz *et al.* through a private communication. Their work is discussed in more detail later in the chapter.

Two checks were carried out on the moduli. With $e_3 = e_1$ the moduli reduce to those given by equations (1.117) and (1.118), for a hydrostatic strain, as is to be expected. The second check involved considering the situation when $e_1 \to 0$, in this case they reduce to those due to a uniaxial compression and so give rise to the moduli in equation (1.120).

The three ratios we require are

$$\frac{C_{33}^*}{C_{44}^*} = \frac{2\left\{\frac{2B}{C}f_2\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}-\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)\right]\right\}}{\left\{\frac{B}{C}\left(\frac{1}{2}f_3\left(\frac{e_3}{e_1}\right)+f_2\left(\frac{e_3}{e_1}\right)\right)\left(\frac{e_3}{e_1}-1\right)-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{e_3}{e_1}-\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)\right\}}, \tag{2.69}$$

$$\frac{C_{11}^*}{C_{66}^*} = \frac{\left\{\frac{B}{C}f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\frac{3}{8}\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{1}{2}-\frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)\right]\right\}}{\left\{\frac{B}{2C}f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\frac{1}{8}\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(-\frac{e_3}{e_1}+\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)\right]\right\}},$$

$$\frac{C_{11}^*}{C_{44}^*} = \frac{2\left\{\frac{B}{C}f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\frac{3}{8}\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{1}{2}-\frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)\right]\right\}}{\left\{\frac{B}{C}\left(\frac{1}{2}f_3\left(\frac{e_3}{e_1}\right)+f_2\left(\frac{e_3}{e_1}\right)\right)\left(\frac{e_3}{e_1}-1\right)-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{e_3}{e_1}-\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)\right\}}$$

and these correspond to three independent $(V_P/V_S)^2$ ratios. As mentioned earlier in this chapter, the first of these corresponds to propagation along the x_3-axis, the second to propagation in the transverse direction with the shear wave polarised in the transverse plane and the third to transverse propagation with shear polarization in the axial direction. The expressions given in equations (2.59), (2.68) and (2.69) are valid for ANY biaxial strain.

The following figures show various plots of the elastic moduli ratios. Figures 2-1, 2-3, 2-5, 2-7, 2-9, 2-10 and 2-11 correspond to Poisson's ratio, $\nu = 1/4$. Figures 2-2, 2-4, 2-6, and 2-8 correspond to Poisson's ratio, $\nu = 1/2$.

In figures 2-1 and 2-2 the elastic moduli ratios are plotted against $k_1\langle\sigma_3\rangle$ and $k_2\langle\sigma_3\rangle$, respectively. For figure 2-1, $k_1\langle\sigma_3\rangle$, is as given in equation (2.61) and the range of values considered is that in which the ratio e_3/e_1 varies from 0 to 7.5. The corresponding range of values for $k_1\langle\sigma_3\rangle$ is $\pi/32$ to 36.3997. For figure 2-2, $k_2\langle\sigma_3\rangle$, is as given in equation (2.63) and the range of values considered is that in which the ratio e_3/e_1 varies from 0 to 13. The corresponding range of values for $k_2\langle\sigma_3\rangle$ is $\pi/32$ to 32.5382. The monotonic increasing curves correspond to equation (2.69a), the essentially horizontal ones to equation (2.69b) and the monotonic decreasing curves to equation (2.69c).

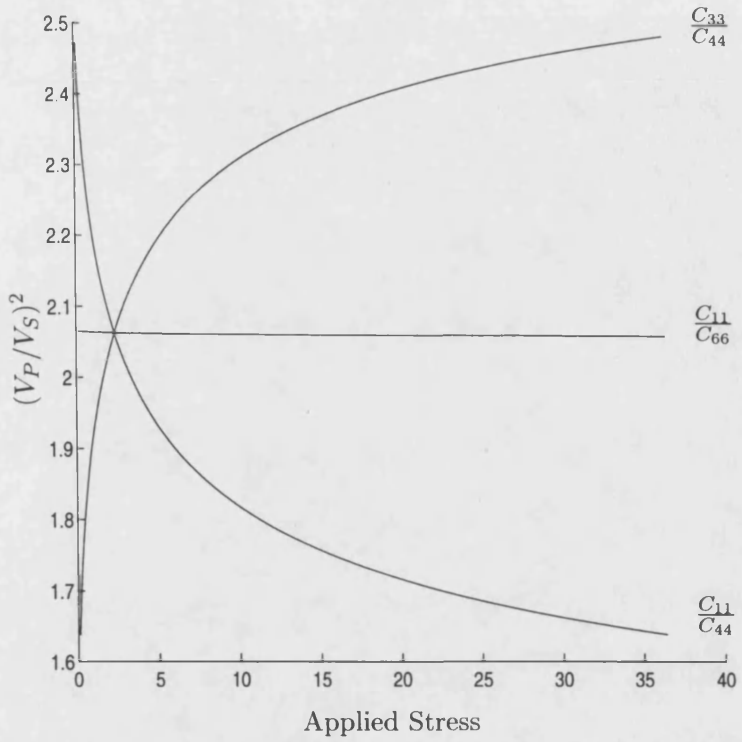

Figure 2-1: *The three (V_P/V_S) ratios versus $k_1 < \sigma_3 >$, Poisson's ratio is 1/4.*

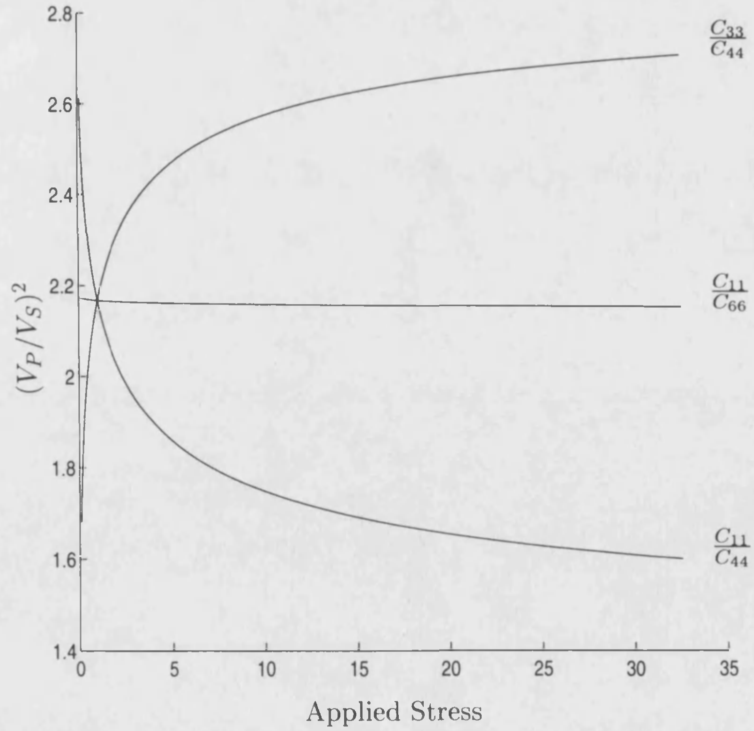

Figure 2-2: *The three (V_P/V_S) ratios versus $k_2 < \sigma_3 >$, Poisson's ratio is 1/2.*

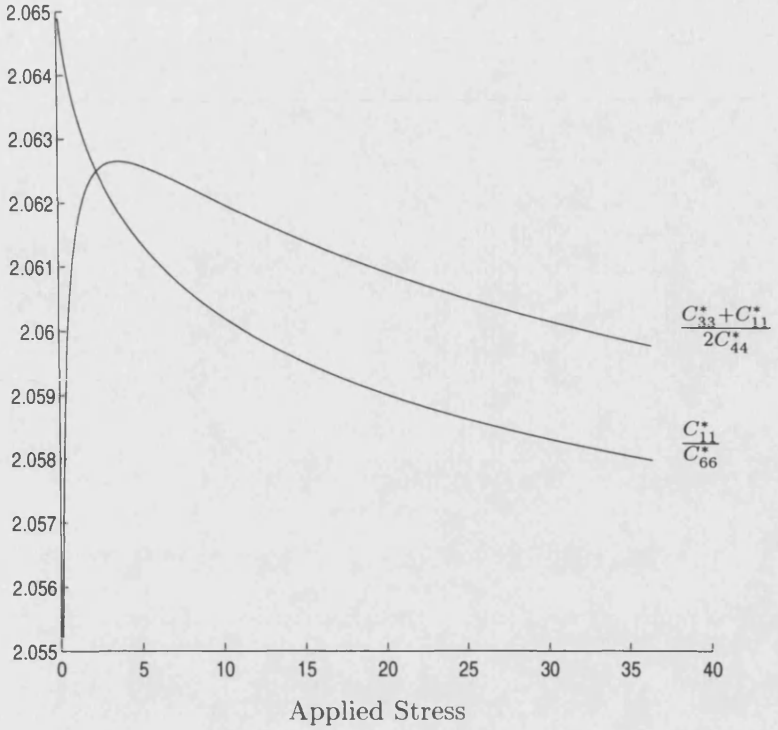

Figure 2-3: *Average of equations (2.69a,c) along with (2.69b) versus* $k_1 < \sigma_3 >$, *Poisson's ratio 1/4.*

In figures 2-1 and 2-2, the point through which all the curves pass is that at which $e_1 = e_3$. These figures suggest that C^*_{11}/C^*_{66} is approximately uniform and that C^*_{33}/C^*_{44} and C^*_{11}/C^*_{44} are symmetrical about some horizontal value. This is considered in more detail in figures 2-3 and 2-4 where the elastic moduli ratio of equation (2.69b) and the average value of the two moduli ratios (2.69a) and (2.69c) are plotted against the third component of applied stress. These two figures show that in fact the average of the two is comparable in value to the third ratio C^*_{11}/C^*_{66}. Also they show more clearly that the value of the ratio C^*_{11}/C^*_{66} does not remain constant but decreases slowly, which is consistent with figure 1 of Schwartz *et al.* [73].

Now in figures 2-5 and 2-6, the three elastic moduli ratios are again plotted, but this time against the additional stress, that is the difference between the stress we have applied and that of the hydrostatic pressure corresponding to $e_3 = e_1$. There obviously appears to be a closer correspondence between these and figure 1 of Schwartz *et al.* [73], than there was with our figures 2-1 and 2-2. However, since we do not know the conditions under which Schwartz' graphs were produced we cannot say whether they should be identical or not.

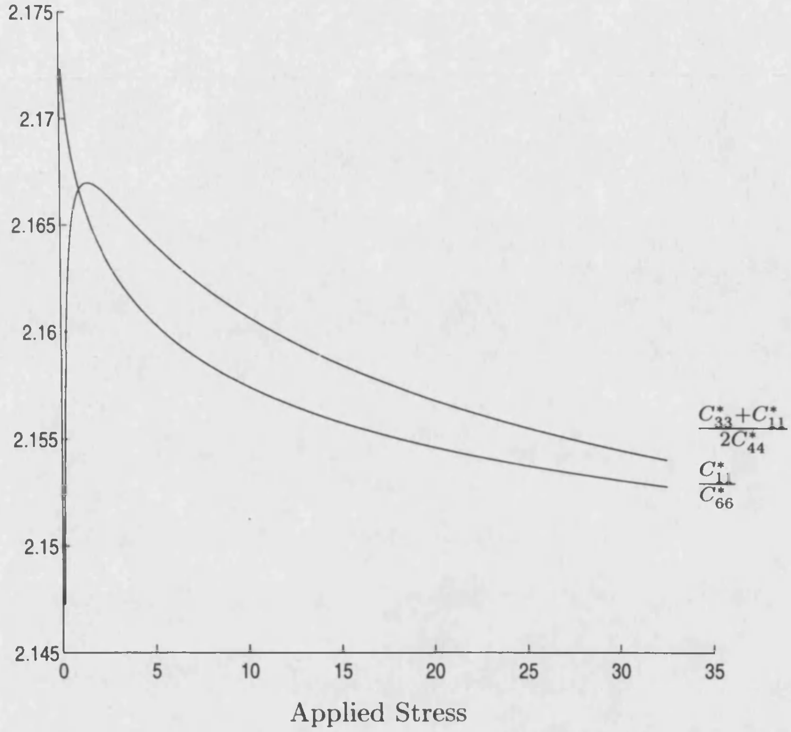

Figure 2-4: *Average of equations (2.69a,c) along with (2.69b) versus $k_2 < \sigma_3 >$, Poisson's ratio 1/2.*

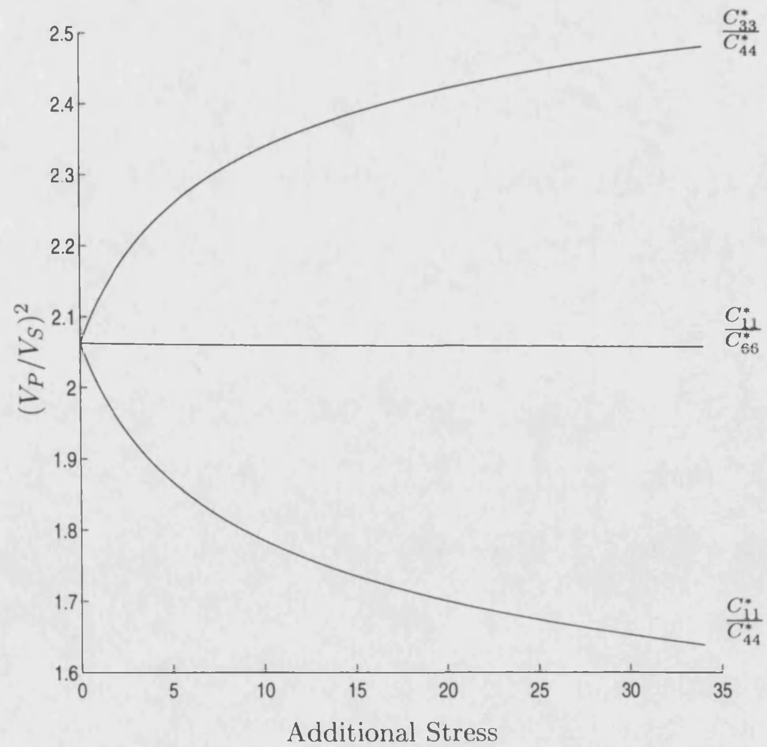

Figure 2-5: *The three (V_P/V_S) ratios versus additional stress, Poisson's ratio is 1/4.*

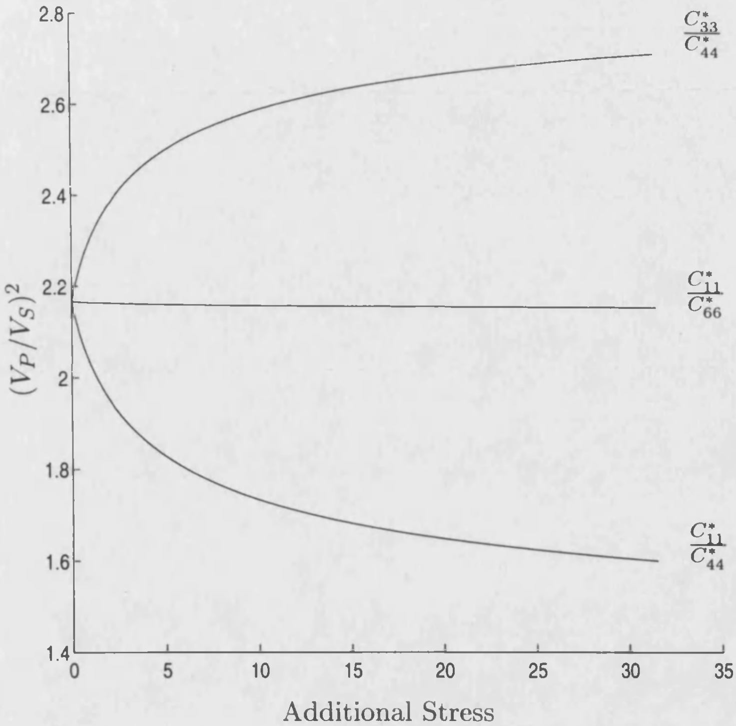

Figure 2-6: *The three (V_P/V_S) ratios versus additional stress, Poisson's ratio is 1/2.*

Figures 2-7 and 2-8 are formed by taking an unnumbered expression given on page 3 of Schwartz *et al.* [73]. This expression gives $\Delta e_3/e$, the increment in hydrostatic pressure, in terms of p_3 which we believe to be the additional stress (see again explanation for figures 2-5 and 2-6),

$$\frac{\Delta e_3}{e} = \frac{0.47 p_3}{(1 + 0.058 p_3)}. \tag{2.70}$$

Then rearranging

$$p_3 = \frac{\Delta e_3/e}{(0.47 - 0.058\Delta e_3/e)} \tag{2.71}$$

and p_3 is plotted along with the additional stress $k_1\langle\sigma_3\rangle - 7/3$ or $k_2\langle\sigma_3\rangle - 7/3$, respectively, against the range of values $e_3/e_1 - 1$ between 0 and 6.5. We subtract 1 from e_3/e_1 as this corresponds to the $\Delta e_3/e$ notation of Schwartz *et al.* [73] and subtract 7/3 from $k_i\langle\sigma_3\rangle$ as this corresponds to the value of the scaled stress for a hydrostatic pressure. The dashed curve is the plot of p_3 in both figures. In fact, p_3 becomes infinite at $\Delta e_3/e = 8.103$ and after that becomes negative, whereas $k_i\langle\sigma_3\rangle$ is continuous and monotonic increasing for all values of $e_3/e_1 - 1$.

Figures 2-9, 2-10 and 2-11 show plots of the elastic moduli ratios C_{33}^*/C_{44}^*, C_{11}^*/C_{66}^* and

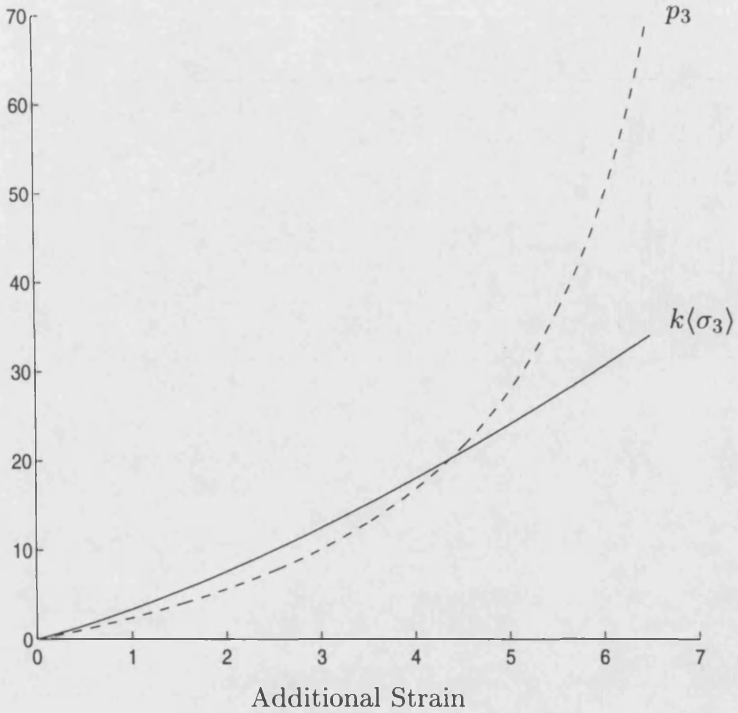

Figure 2-7: *Additional stress and* $k_1 < \sigma_3 >$ *versus the additional strain, Poisson's ratio 1/4.*

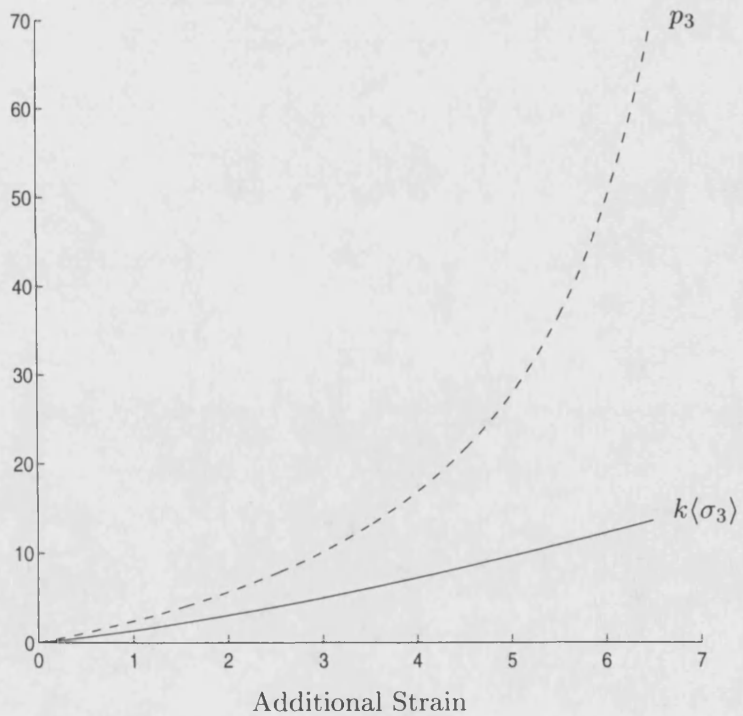

Figure 2-8: *Additional stress and* $k_2 < \sigma_3 >$ *versus the additional strain, Poisson's ratio 1/2.*

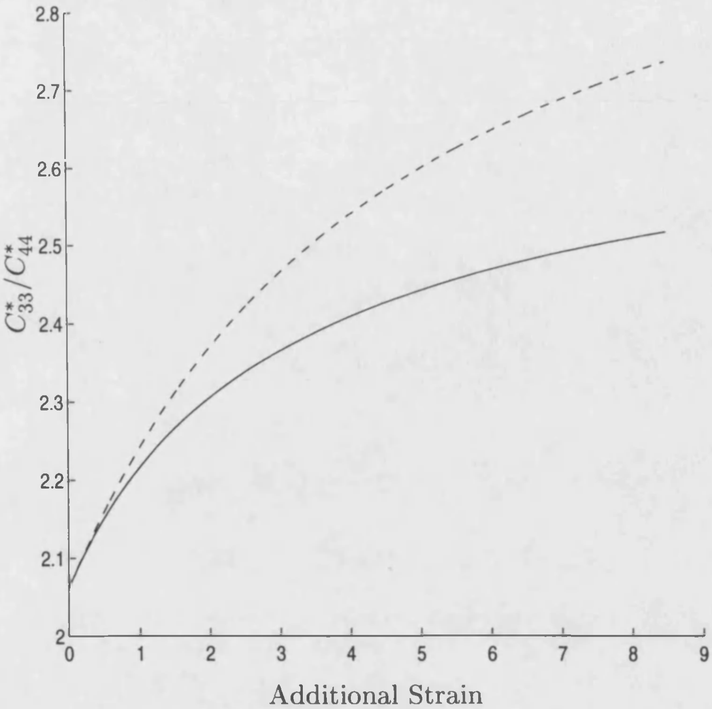

Figure 2-9: *Comparing the values of our modulus C_{33}^*/C_{44}^* with those of Schwartz et al. [73]*

C_{11}^*/C_{44}^* respectively, for both the moduli given in equations (13)-(17) of Schwartz *et al.* [73] and those given in equation (2.69) of this work, against $e_3/e_1 - 1$. The dashed lines represent the Schwartz *et al.* [73] ratios. For small values of $e_3/e_1 - 1$, which is what is considered in Schwartz *et al.* [73], each graph shows that the two ratio plots take values that correspond very closely. However, although the shapes are clearly similar, there is no overall correspondence between the two plots.

Unfortunately, it is difficult to compare anything other than the shape of the curves with those of figure 1 of Schwartz *et al.* [73]. We do not know whether the values of stress used to obtain figure 1 in Schwartz *et al.* [73] are incremental values or not. For figures 2-1 and 2-2 which correspond to actual applied stress, we cannot even find a positive value of e_3/e_1 that gives a value of zero stress and so we will not be able to start these as figure 1 of Schwartz *et al.* [73] does.

Further comparisons could also be made if we knew the value of Poisson's ratio used to obtain figure 1 of Schwartz *et al.* [73]. Taking larger values of Poisson's ratio raises the initial value of our ratios, but even by taking $\nu = 1/2$, we cannot raise our starting value to that of fractionally above 2.2 as is the case in figure 1 of Schwartz *et al.* [73].

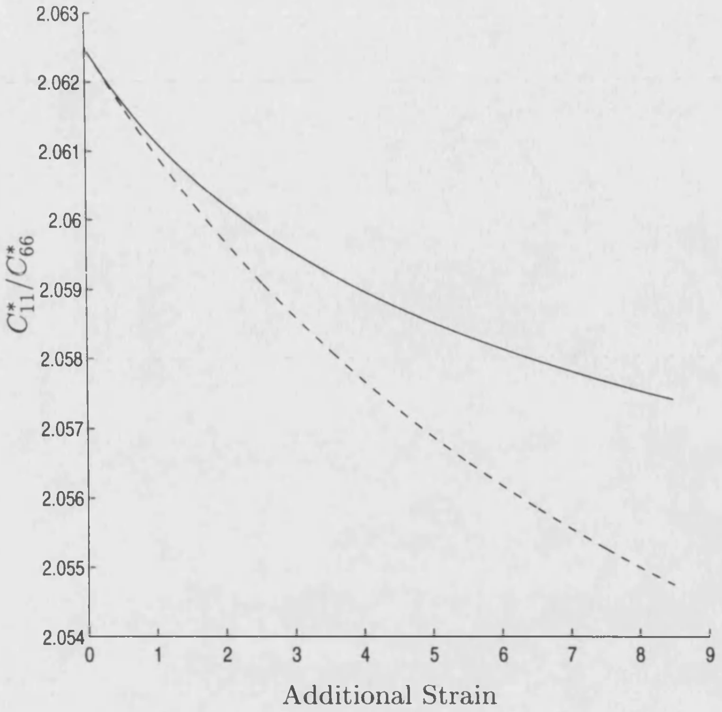

Figure 2-10: *Comparing the values of our modulus C^*_{11}/C^*_{66} with those of Schwartz et al. [73]*

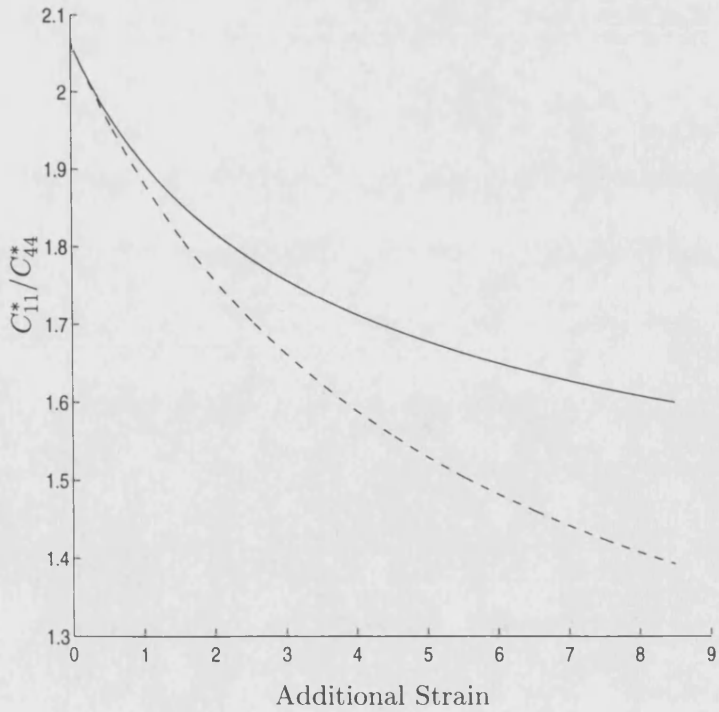

Figure 2-11: *Comparing the values of our modulus C^*_{11}/C^*_{44} with those of Schwartz et al. [73]*

Our work suggests that to allow us to take a value of approximately 2.2 for our ratios when there is zero stress, we would need to take $\nu = 5/9$ which we know is physically impossible for real materials. Even the initial values of the ratios found from Schwartz *et al.* [73] do not reach 2.2 as they will clearly be equal to those of our ratios and the hydrostatic case, that is 33/16 for $\nu = 1/4$ and 13/6 for $\nu = 1/2$.

Since there is such a lack of information in the work of Schwartz *et al.* [73] our problem throughout is that it is impossible to draw any firm conclusions upon comparison with our new results. As mentioned above, we have tried varying Poisson's ratio to reproduce their results. However, it would seem that the best we can do is say that our figures 2-5 and 2-6 appear to be consistent with figure 1 of Schwartz *et al.* [73].

2.3.3 Recalculation of the Effective Elastic Moduli with the Inclusion of Sphere Rotations

As we have already seen, in chapter 2 of Slade [76] the equilibrium of a sphere in a random packing is investigated. Equations for the equilibrium of the sum of all the incremental forces and the sum of the moments are reduced to expressions that we can use here as we recalculate the elastic moduli and their ratios including the effects of individual sphere rotations. These rotations do not effect the expressions for the average stress found by considering the initial deformation. The stress is thus given by equations (2.59) and (2.66) for infinitely rough and perfectly smooth spheres respectively.

The condition for equilibrium of moments can be written as an average over all the spheres, provided the packing is dense enough and reduces to equation (1.149):

$$\left\langle (-e_{pq}I_pI_q)^{1/2}(\delta_{ik} - I_iI_k)\right\rangle \delta\omega_k = \epsilon_{irk}\left\langle (-e_{pq}I_pI_q)^{1/2}I_rI_l\right\rangle \delta e_{kl}. \tag{2.72}$$

We can find the rotation vector $\delta\omega$ for our initial strain field from this equation and subsequently find $\langle\delta\sigma_{ij}\rangle$ as given by equation (1.152):

$$\begin{aligned}\langle\delta\sigma_{ij}\rangle \;=\; & \frac{3\phi\eta}{2\pi^2 B(2B+C)}\left\{C\left\langle (-e_{pq}I_pI_q)^{1/2}I_iI_jI_kI_l\delta e_{kl}\right\rangle\right. \qquad (2.73)\\ & \left. +2B\left\langle (-e_{pq}I_pI_q)^{1/2}I_lI_i\delta e_{jl}\right\rangle - 2B\epsilon_{jkl}\left\langle (-e_{pq}I_pI_q)^{1/2}I_iI_l\delta\omega_k\right\rangle\right\}\end{aligned}$$

from which we can determine the effective elastic moduli.

We have our initial strain given by

$$e_{ij} = e_1(\delta_{i1}\delta_{j1} + \delta_{i2}\delta_{j2}) + e_3\delta_{i3}\delta_{j3} \tag{2.74}$$

and so in this case equation (2.72) yields

$$\left\langle(-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}(\delta_{ik} - I_iI_k)\right\rangle\langle\delta\omega_k\rangle = \epsilon_{irk}\left\langle(-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}I_rI_l\right\rangle\langle\delta e_{kl}\rangle \tag{2.75}$$

and we again have to evaluate integrals of the kind mentioned earlier and seen in equation (2.54). Taking $i = 1, 2, 3$ in turn, we obtain the components of the rotation tensor in terms of the previously defined functions f_1, f_2, and f_3,

$$\begin{aligned} \delta\omega_1 &= \frac{f_3(e_3/e_1) - 2f_2(e_3/e_1)}{2f_1(e_3/e_1) - f_3(e_3/e_1)}\delta e_{23} \\ \delta\omega_2 &= \frac{2f_2(e_3/e_1) - f_3(e_3/e_1)}{2f_1(e_3/e_1) - f_3(e_3/e_1)}\delta e_{13} \\ \delta\omega_3 &= 0. \end{aligned} \tag{2.76}$$

Now the incremental stress from equation (2.73) is

$$\begin{aligned} \langle\delta\sigma_{ij}\rangle = \frac{3\phi\eta}{2\pi^2B(2B+C)}\Big\{&C\left\langle((-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}I_iI_jI_kI_l\delta e_{kl}\right\rangle \\ &+2B\left\langle(-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}I_lI_i\delta e_{jl}\right\rangle \\ &-2B\epsilon_{jkl}\left\langle(-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}I_iI_l\delta\omega_k\right\rangle\Big\} \end{aligned} \tag{2.77}$$

Taking i=j=1 in the above yields

$$\begin{aligned} \langle\delta\sigma_{11}\rangle = \frac{3\phi\eta}{2\pi^2B(2B+C)}\Big\{&C\left\langle((-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}I_1^2I_kI_l\delta e_{kl}\right\rangle \\ &+2B\left\langle(-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}I_lI_1\delta e_{1l}\right\rangle\Big\} \end{aligned} \tag{2.78}$$

from which we find

$$\begin{aligned} C_{11}^* &= \frac{3\phi\eta(-e_1)^{1/2}}{4\pi^2B(2B+C)}\left\{Bf_3\left(\frac{e_3}{e_1}\right) + \frac{3}{8}C\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(\frac{1}{2} - \frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)} + f_3\left(\frac{e_3}{e_1}\right)\right]\right\} \\ C_{13}^* &= \frac{3\phi\eta C(-e_1)^{1/2}}{8\pi^2B(2B+C)}\left\{\frac{-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(-\frac{1}{2} + \frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1} - 1\right)}\right\}. \end{aligned} \tag{2.79}$$

Similarly, the rotation term is zero in both $\langle\delta\sigma_{33}\rangle$ and $\langle\delta\sigma_{12}\rangle$ and so

$$C_{33}^{*} = \frac{3\phi\eta(-e_1)^{1/2}}{4\pi^2 B(2B+C)}\left\{2Bf_2\left(\frac{e_3}{e_1}\right)+C\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}-\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1}-1\right)}\right]\right\} \tag{2.80}$$

$$C_{66}^{*} = \frac{3\phi\eta(-e_1)^{1/2}}{4\pi^2 B(2B+C)}\left\{\frac{B}{2}f_3\left(\frac{e_3}{e_1}\right)+\frac{C}{8}\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(-\frac{e_3}{e_1}+\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1}-1\right)}+f_3\left(\frac{e_3}{e_1}\right)\right]\right\}.$$

These last four are identical to those found previously in equation (2.68). However, taking i=1 and j=3 the rotation term is non-zero,

$$\begin{aligned}\langle\delta\sigma_{13}\rangle = \frac{3\phi\eta}{2\pi^2 B(2B+C)}&\left\{C\left\langle((-e_1\sin^2\theta-e_3\cos^2\theta)^{1/2}I_1I_3I_kI_l\delta e_{kl}\right\rangle\right.\\&+2B\left\langle(-e_1\sin^2\theta-e_3\cos^2\theta)^{1/2}I_lI_1\delta e_{3l}\right\rangle\\&\left.-2B\epsilon_{3pq}\left\langle(-e_1\sin^2\theta-e_3\cos^2\theta)^{1/2}I_1I_q\delta\omega_p\right\rangle\right\}\end{aligned} \tag{2.81}$$

and the fifth modulus is calculated to be

$$C_{44}^{*} = \frac{3\phi\eta(-e_1)^{1/2}}{8\pi^2 B(2B+C)}\left\{4B\frac{f_2\left(\frac{e_3}{e_1}\right)f_3\left(\frac{e_3}{e_1}\right)}{2f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)}+C\left[\frac{-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{e_3}{e_1}-\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)}{\left(\frac{e_3}{e_1}-1\right)}\right]\right\}. \tag{2.82}$$

This is not the same as the expression for C_{44}^{*} that we found in equation (2.68). We can do a check on this modulus by considering $e_3 = e_1$ when the modulus reduces to that of the hydrostatic case. Figure 2-12 shows a plot of the ratio of the two expressions for the C_{44}^{*} moduli found without and with the inclusion of rotations. Since the value of the ratio is always ≥ 1, the modulus calculated without using the rotations must always takes a value greater than or equal to the value of that found with the inclusion of rotations.

The first and third of the three required ratios are effected by the inclusion of rotations, the second is not. Since Schwartz *et al.* [73] did not consider rotations in their work then upon application of a perturbed hydrostatic strain the only ratio that will be identical with those derived in Schwartz' work will be the second. Using the new expressions for

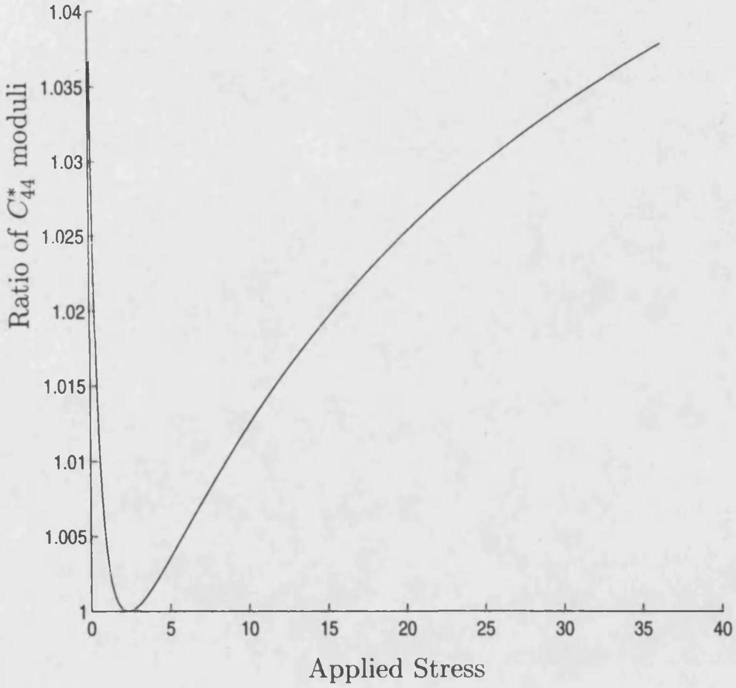

Figure 2-12: *Ratio of equations (2.68e) and (2.82) versus applied stress, Poisson's ratio 1/4.*

our moduli, we now have

$$\begin{aligned}
\frac{C^*_{33}}{C^*_{44}} &= \frac{2\left\{\frac{2B}{C}f_2\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}-\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)\right]\right\}}{\left\{\frac{4B}{C}\frac{f_2\left(\frac{e_3}{e_1}\right)f_3\left(\frac{e_3}{e_1}\right)}{2f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)}\left(\frac{e_3}{e_1}-1\right)-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{e_3}{e_1}-\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)\right\}} \qquad (2.83)\\
\frac{C^*_{11}}{C^*_{66}} &= \frac{\left\{\frac{B}{C}f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\frac{3}{8}\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{1}{2}-\frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)\right]\right\}}{\left\{\frac{B}{2C}f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\frac{1}{8}\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(-\frac{e_3}{e_1}+\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)\right]\right\}}\\
\frac{C^*_{11}}{C^*_{44}} &= \frac{2\left\{\frac{B}{C}f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)+\frac{3}{8}\left[\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{1}{2}-\frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)\left(\frac{e_3}{e_1}-1\right)\right]\right\}}{\left\{\frac{4B}{C}\frac{f_2\left(\frac{e_3}{e_1}\right)f_3\left(\frac{e_3}{e_1}\right)}{2f_2\left(\frac{e_3}{e_1}\right)+f_3\left(\frac{e_3}{e_1}\right)}-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{e_3}{e_1}-\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)\right\}}.
\end{aligned}$$

Figure 2-13 has 2 plots of the ratios with Poisson's ratio equal to 1/4. One plot includes the effects of individual sphere rotations, this is represented by the dashed line, while the other is a plot of the ratios considered in the previous section. We can see that with the inclusion of rotations the ratios C^*_{33}/C^*_{44} and C^*_{11}/C^*_{44} no longer appear symmetrical about the other ratio C^*_{11}/C^*_{66}.

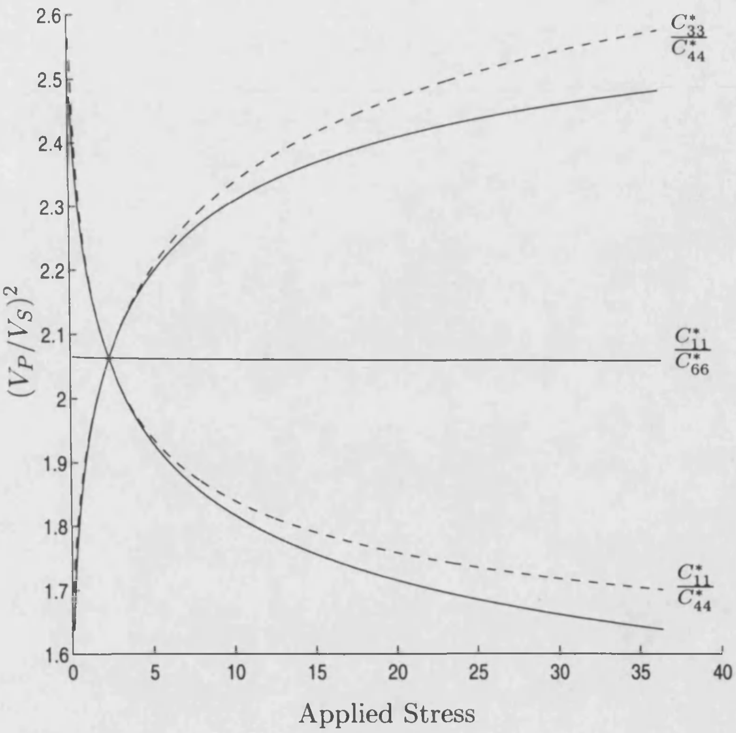

Figure 2-13: *Comparing the (V_P/V_S) ratios with and without the effects of sphere rotations*

2.4 Path Dependent Results

Shortly after completing this work, we received a communication from Lawrence Schwartz. He, in conjunction with several other authors, has also done some work to calculate the effective elastic moduli for a general biaxial strain, when the spheres in the packing are infinitely rough, Johnson *et al.* [45]. In the work they show that the expression for the moduli, equation (2.10) of this chapter and derived by Walton [86], is valid for any applied strain and independent of the history of the medium. That is, the expressions for the moduli are path independent, they depend only upon the present state of deformation, that is the current state of strain but not upon how it was reached. Contrasting with this, Johnson *et al.* [45] also show that the elements of stress are explicitly path dependent. They illustrate this by considering three different cases of a combined hydrostatic and uniaxial strain.

In the analysis of Walton [86], it was assumed that the normal and tangential strain components increased in direct proportion to one another. Johnson *et al.* [45], however, refer to a paper written recently by Norris and Johnson [60]. In this latter paper, $2w$

is the relative approach of the two spheres along the line joining their centres. The relative tangential displacement between the two spheres is $2s$. The force is decomposed into a normal force N and a tangential force T. A small change in displacement (δw, δs), leads to a small change in the restoring force (δN, δT) and all models considered can be written in the form:

$$\delta N = C_n a_n(w)\delta w, \;\; \delta T = C_t a_t(w)\delta s. \tag{2.84}$$

We are only concerned with Hertzian contacts and so

$$a_n(w) = a_t(w) = (Rw)^{1/2}. \tag{2.85}$$

It was Norris and Johnson [60], who initially found the expression for the second order elastic moduli associated with incremental displacements around a given state that is used by Johnson *et al.* [45]. It does depend upon the current state of strain but not upon the strain history of the medium. Their expressions are identical to those given by equation (2.10). However, as mentioned above the problem of finding the work done to bring a single contact to a given strain state is obviously path dependent and path dependent effects are well known in granular media. In his work, Deresiewicz [26] and [27], for example, has considered the effects when the packing is a simple cubic array of particles.

This would imply that although we also assumed that the strain components increased in direct proportion to one another when deriving our elastic moduli in this chapter, these results are valid for any strain history of the granular packing. Comparing our expressions for the elastic moduli, with those derived by Johnson *et al.* [45], we see that the results are in agreement.

To compare their results with experiment, Johnson et al. [45] calculate an expression for the stress tensor in terms of the strain. It is experimentally difficult to measure the strain in an unconsolidated sample, often it is the stress components that are measured, hence the need for this relationship. The three strain paths they consider are shown in figure 2-14. In all three of these cases the stress has the form

$$(\langle\sigma_{ij}\rangle) = \mathrm{diag}\;\; (\langle\sigma_1\rangle, \langle\sigma_1\rangle, \langle\sigma_3\rangle). \tag{2.86}$$

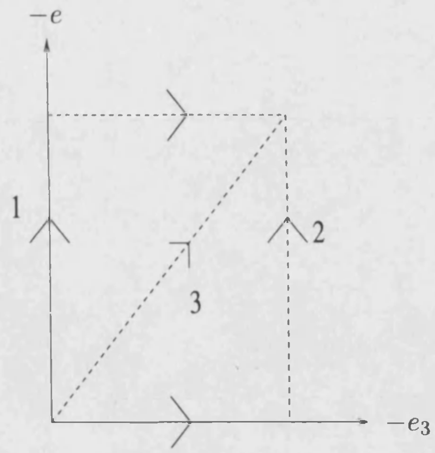

Figure 2-14: *Strain paths*

Given below are the expressions Johnson *et al.* [45] found for the stress tensor, related to each strain path. We have rewritten their results in our notation for ease of comparison. In path 1, the system is first hydrostatically compressed and then an additional uniaxial compression is applied. Their stress expressions were calculated using equation (13) of their communication:

$$
\begin{aligned}
<\sigma_1> &= -\frac{\phi n(-e_1)^{3/2}}{2\pi^2 B(2B+C)}\left\{\frac{4}{3}B\left(\frac{e_1}{e_3-e_1}\right)^{3/2}\right. \\
&\qquad \left. +C\left(f_1\left(\frac{e_3}{e_1}\right)+\left(\frac{e_3}{e_1}-\frac{3}{2}\right)f_2\left(\frac{e_3}{e_1}\right)-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}\right)\right\}, \\
<\sigma_3> &= -\frac{\phi n(-e_1)^{3/2}}{2\pi^2 B(2B+C)}\left\{2B\left(f_1\left(\frac{e_3}{e_1}\right)+\left(\frac{e_3}{e_1}-1\right)f_2\left(\frac{e_3}{e_1}\right)-\frac{2}{3}\left(\frac{e_1}{e_3-e_1}\right)^{3/2}\right)\right. \\
&\qquad \left. +C\left(\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}\right)\right\}. \qquad (2.87)
\end{aligned}
$$

In the second path shown in figure 2-13, a uniaxial compression is followed by an hydrostatic compression. The stress is now given by:

$$
\begin{aligned}
<\sigma_1> &= -\frac{\phi n(-e_1)^{3/2}}{4\pi^2 B(2B+C)}\left\{2B\left(-\frac{1}{6}+f_1\left(\frac{e_3}{e_1}\right)+\left(\frac{e_3}{e_1}-\frac{3}{2}f_2\left(\frac{e_3}{e_1}\right)-\frac{1}{3}(\frac{e_3}{e_1})^{3/2}\right)\right)\right. \\
&\qquad \left. +C\left(f_1\left(\frac{e_3}{e_1}\right)+\left(\frac{e_3}{e_1}-\frac{3}{2}\right)f_2\left(\frac{e_3}{e_1}\right)-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}\right)\right\}, \\
<\sigma_3> &= -\frac{\phi n(-e_1)^{3/2}}{4\pi^2 B(2B+C)}\left\{2B\left(\frac{1}{3}+f_2\left(\frac{e_3}{e_1}\right)+\frac{2}{3}\left(\frac{e_3}{e_1}\right)^{3/2}\right)\right. \\
&\qquad \left. +C\left(f_2\left(\frac{e_3}{e_1}\right)+\frac{2}{3}\left(\frac{e_3}{e_1}\right)^{3/2}\right)\right\} \qquad (2.88)
\end{aligned}
$$

Finally, for the third path, the two components are applied together as they were in our calculations and

$$\begin{aligned}
< \sigma_1 > &= -\frac{\phi n(-e_1)^{3/2}}{4\pi^2 B(2B+C)}\left\{(2B+\frac{3C}{4})f_1\left(\frac{e_3}{e_1}\right)-(2B+\frac{C}{2})f_2\left(\frac{e_3}{e_1}\right)+\frac{C}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\}, \\
< \sigma_3 > &= -\frac{\phi n(-e_1)^{3/2}}{\pi^2 B(2B+C)}\left\{(\frac{Be_3}{e_1}+\frac{C}{4})f_2\left(\frac{e_3}{e_1}\right)+\frac{C}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\}. \qquad (2.89)
\end{aligned}$$

As we would expect, this third set of results is identical to those we found (see equation (2.59)).

Johnson *et al.* [45], plot the stress components for the different strain paths considered and conclude that the differences between the three sets of curves is quite small. Their work shows that the relationship between stress and strain is path dependent, even though the moduli are path independent.

Chapter 3

A Perturbation of the Uniform Strain Approximation

3.1 Comparison Between Experimental Results, Numerical Simulations and Theoretical Predictions

In their paper, Jenkins *et al.* [43] discuss three approaches to finding the effective elastic moduli of a packing of glass spheres - experimental studies, numerical simulations and theoretical predictions. They conclude that there is an apparent failure on the part of the theoretical approach in predicting numerical values for the effective shear and bulk moduli, under an initial hydrostatic confining pressure. In this and the following chapters, we highlight the differences between the approaches and then attempt to modify the theory to incorporate these differences. In this way, we obtain revised predictions for the effective moduli.

The experiments considered by Jenkins *et al.* [43] were carried out in a true triaxial/torsional device, in the form of a column. A variety of stress paths and loading histories were imposed. The results for further stress paths and loading histories are presented in both the paper by Chen *et al.* [17] and that by Ishibashi *et al.* [42]. These also give detailed descriptions of the experimental apparatus and method used.

The experimental set-up consisted of a hollow cylindrical sample containing a binary packing of glass spheres and water. The diameters of the larger of the two sizes of spheres were between 0.300-0.425mm and the smaller between 0.180-0.250mm, with around ten small spheres to one large sphere. The shear modulus of the glass was 3.0x10^7kPa, Poisson's ratio, $\nu = 0.21$, the specific gravity (density/density of water) was 2.5 and the coefficient of friction f between contacts measured to be 0.3.

The sample was brought to an initial porosity of 0.37 and the isotropic mean stress increased to 138kPa. The pressure was held fixed and deviatoric loading applied. We are purely interested in the values of the effective bulk and shear moduli. The value for the former is not given in the experimental data, but for the latter was found to be 161MPa at the initiation of the shearing.

The numerical simulations were conducted using a distinct element method (DEM) that involved solving the equations of motion to find the displacements and rotations for a binary packing of spheres. The forces acting across the contact areas between spheres depend upon their geometry, elasticity and friction through a Coulomb-type friction law. Cundall and Strack [24] describe this DEM. The simulation was run on a periodic cell, so that any boundary effects would be eliminated. The sample consisted of 432 spheres, 392 of which had radius 0.1075mm and 40 of which had radius 0.1825mm. The initial porosity was 0.368 and an isotropic stress of 138 kPa was again applied.

More detailed explanations about the simulations are given in Cundall [20] and [21]. Cundall *et al.* [23], also describes the adjustments that need to be made to achieve the same porosity, at the same pressure as those in the experiments. However, this is as far as the similarity between initial conditions extends. In the experiments, the initial value for the shear modulus was measured from an initial state that was anisotropic due to the boundary effects. In the simulations there was an isotropic initial state and the calculated effective shear modulus before any shearing was applied to the cell was found to be 127MPa.

The theory considered for comparison is the work of Walton [86], that is the uniform strain approximation discussed in the introductory chapter of this thesis. From the theory the value for the effective shear modulus was calculated to be 338MPa, almost three times that found by the numerical simulation and twice that in the experiment. Also, calculating the effective bulk modulus the theory yielded a value of 245MPa, whereas the numerical simulations a value of 185MPa.

The numerical simulations and theory would appear to have the same initial conditions, so why this large discrepancy between the values for the effective moduli? As we have already mentioned, this is the first of three chapters in which we set about to try and bring closer correlation between these approaches and to suggest some reasons why we might not expect them to be identical anyway. In this first chapter, we perturb the work of Walton [86], the uniform strain approximation, described in Chapter 1.

We are particularly interested in bringing closer correlation between the values predicted by the numerical simulation and the theory. The experimental conditions will not be exactly reproduced by either the numerical simulations or this particular theory as the experimental sample can never be truly isotropic. This is due to the boundary conditions that exist because of the walls of the sample container.

Two further papers by Cundall *et al.* [22] and Cundall and Strack [25], may hold part of the answer as to why the numerical simulations and theory give inconsistent results. The papers describe further results from the computer program BALL which is used for comparison in Jenkins *et al.* [43]. Both papers note that one of the microscopic observations made on the simulated packing is that forces are concentrated in chains of particles. They are never transmitted across a sample in a uniform way, so some particles may carry little or no load, while others take a substantial amount of load. Figure 1 of Cundall and Strack [25], shows a diagram of how these force chains might arise in a simulation.

The uniform strain approximation cannot incorporate this feature of the numerical simulation. After the application of an initial hydrostatic compression, $e_{ij} = e\delta_{ij}$, we saw in Chapter 1 that under the assumption of uniform strain approximation, the force acting across a contact area is given by:

$$\mathbf{F}^{(nn')} = -\frac{4R^2(-e)^{3/2}}{3\pi B}\mathbf{I}^{(nn')} \tag{3.1}$$

where R is the radius of the spheres. The magnitude of this will be the same at any contact throughout the packing. However, if we perturb the uniform strain approximation, it may be possible that we will find a variation in the forces across the contact areas. Unfortunately, we will still not know whether these occur in the chains that we see in the numerical simulation.

3.2 Correction Terms in the Uniform Strain Approximation

3.2.1 The Initial Deformed State

We proceed as in previous chapters by first considering the packing as a whole and impose an initial confining displacement on the boundary. This displacement takes the form

$$u_i = e_{ij}x_j. \tag{3.2}$$

Thus it is consistent with a uniform compressive strain and e_{ij} are the components of a symmetric constant tensor. In the undeformed material, the position vector of the centre of a typical sphere n is denoted by $X_j^{(n)}$. After the deformation, the centre of this sphere will have been displaced, let this displacement be $u_i^{(n)}$ and its rotation, about an axis through its centre, be $\omega_i^{(n)}$.

We initially restrict our attention to the case of infinitely rough spheres, the results for those that are perfectly smooth will be given later. We can use the general expression given by equation (1.125), to calculate the force acting on the nth sphere due to its contact with the n'th, that is

$$\begin{aligned} F_i^{(nn')} &= \frac{(2R)^{1/2}}{3\pi B(2B+C)}\left\{2B[(u_p^{(n')}-u_p^{(n)})I_p^{(nn')}]^{1/2}\right. \\ &\quad \left. x(u_i^{(n')}-u_i^{(n)}+R\epsilon_{ijk}(\omega_j^{(n')}+\omega_j^{(n)})I_k^{(nn')})+C[(u_p^{(n')}-u_p^{(n)})I_p^{(nn')}]^{3/2}I_i^{(nn')}\right\}, \end{aligned} \tag{3.3}$$

where R is the radius of each sphere and B and C are the constants, previously defined, that can be written as combinations of the Lamé moduli. We have the unit vector directed along the line of centres, $I_i^{(nn')}$, defined as:

$$I_i^{(nn')} = \frac{X_i^{(n)} - X_i^{(n')}}{2R}. \tag{3.4}$$

To determine this force we again have to make some kind of assumption about the relative displacement $(u_i^{(n')} - u_i^{(n)})$ and the relative rotation $(\omega_i^{(n)} + \omega_i^{(n')})$. We have already seen that, Walton [86] assumes that the displacement of the sphere centres is consistent with the applied uniform field. Thus

$$u_i^{(n)} = e_{ij} X_j^{(n)}, \tag{3.5}$$

and also that the rotation of each sphere about an axis through its centre is the same. Thus

$$\omega_i^{(n)} = \Omega_i. \tag{3.6}$$

These last two equations constitute the uniform strain approximation.

As a first attempt to modify the theory and hence improve the correlation between theoretical predictions and the numerical simulation results, we consider perturbations $\tilde{u}_i^{(n)}$ and $\tilde{\omega}_i^{(n)}$ of the rigid-body translation and rotation about an axis through the sphere centre, respectively. Then for the nth sphere, we have that

$$u_i^{(n)} = e_{ij} X_j^{(n)} + \tilde{u}_i^{(n)} \tag{3.7}$$

and

$$\omega_i^{(n)} = \Omega_i + \tilde{\omega}_i^{(n)}. \tag{3.8}$$

We consider the calculations for initial hydrostatic conditions as we only have numerical simulation data for such a compression. This gives us $\Omega_i = 0$ and then

$$\omega_i^{(n)} = \tilde{\omega}_i^{(n)}$$

and also

$$e_{ij} = e\delta_{ij}.$$

3.2.2 Equilibrium Conditions

In order to find approximations for any of the perturbations when the initial deformation has any of the forms mentioned above, we consider the equilibrium of forces and moments on the nth sphere. We require that the sum of all the forces and also that of the moments be zero. Thus

$$\sum_{n'} F_i^{(nn')} \quad = \quad 0,$$

$$\sum_{n'} \epsilon_{ijk} I_j^{(nn')} F_k^{(nn')} = 0 \tag{3.9}$$

where the summations are over all spheres n' in contact with the nth sphere.

For large co-ordination values, that is, each sphere has a large number of contacts, we would expect the uniform strain approximation to accurately predict the displacement of the centre of the nth sphere upon application of a confining force. However, as the co-ordination number decreases the error in the approximation increases. The work of Walton [86], which is based upon this assumption has already been discussed in Section 1.3.2. However, the conditions for equilibrium of the nth sphere are given in equations (3.9). Using the expression for $\mathbf{F}^{(nn')}$ given in equation (3.1), obtained using the uniform strain approximation, these will be satisfied exactly provided

$$\sum_{n'} \mathbf{I}^{(nn')} = \mathbf{0}. \tag{3.10}$$

Summation is over all spheres n' in contact with the nth sphere and if each sphere has a large co-ordination number then we would expect this last equation to be a good approximation. However, with decreasing co-ordination number the approximation becomes worse and so here we have modified the assumptions.

We calculate the force acting on the nth sphere due to its contact with the n'th, using equation (3.3). We must first expand the terms $[(u_p^{(n')} - u_p^{(n)})I_p^{(nn')}]^{1/2}$ and $[(u_p^{(n')} - u_p^{(n)})I_p^{(nn')}]^{3/2}$ using the binomial expansion. In the case of an initial hydrostatic compression, $e_{ij} = e\delta_{ij}$ and since $u_i^{(n)} = e_{ij}X_j + \tilde{u}_i^{(n)}$ then also using the fact that $I_p^{(nn')} I_p^{(nn')} = 1$, the first terms in the expansion of each are as follows:

$$\begin{aligned}[(u_p^{(n')} - u_p^{(n)})I_p^{(nn')}]^{1/2} &= (-2Re)^{1/2}\left(1 - \frac{1}{4Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})I_p^{(nn')}\right. \\ &\left. -\frac{1}{32R^2e^2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)})I_p^{(nn')}I_q^{(nn')}\right) + O((\tilde{u}_p^{(n')})^3)\end{aligned} \tag{3.11}$$

and

$$\begin{aligned}[(u_p^{(n')} - u_p^{(n)})I_p^{(nn')}]^{3/2} &= (-2Re)^{3/2}\left(1 - \frac{3}{4Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})I_p^{(nn')}\right. \\ &\left. +\frac{3}{32R^2e^2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)})I_p^{(nn')}I_q^{(nn')}\right) + O((\tilde{u}_p^{(n')})^3).\end{aligned} \tag{3.12}$$

We also have $\Omega_i = 0$ and hence upon substitution of this and equations (3.11) and (3.12) into equation (3.3), we see that

$$\begin{aligned} F_i^{(nn')} &= \frac{2R(-e)^{1/2}}{3\pi B(2B+C)} \left[1 - \frac{1}{4Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)}) I_p^{(nn')} \right. \\ & \left. - \frac{1}{32R^2e^2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)}) I_p^{(nn')} I_q^{(nn')} \right] \\ & x \left\{ 2B \left(-2ReI_i^{(nn')} + (\tilde{u}_i^{(n')} - \tilde{u}_i^{(n)}) + \epsilon_{ikl} R I_l^{(nn')} (\omega_k^{(n')} + \omega_k^{(n)}) \right) \right\} \\ & \quad +2RC(-e) \left[1 - \frac{1}{2Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)}) I_p^{(nn')} \right. \\ & \left. + \frac{3}{32R^2e^2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)}) I_p^{(nn')} I_q^{(nn')} \right] I_i^{(nn')} + O((\tilde{u}_p^{(n')})^3). \end{aligned} \tag{3.13}$$

Substituting this general expression for $F_i^{(nn')}$ into the first of the equilibrium conditions, equation (3.9a) and retaining only terms of order $\tilde{u}_i^{(n)}\tilde{u}_j^{(n)}$ or lower, we obtain:

$$\begin{aligned} & \textstyle\sum_{n'} B \Big(-2ReI_i^{(nn')} + \tilde{u}_i^{(n')} - \tilde{u}_i^{(n)} + \epsilon_{ikl} R I_l^{(nn')} (\tilde{\omega}_k^{(n')} + \tilde{\omega}_k^{(n)}) + \tfrac{1}{2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)}) I_p^{(nn')} I_i^{(nn')} \\ & - \tfrac{1}{4Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_i^{(n')} - \tilde{u}_i^{(n)}) I_p^{(nn')} - \tfrac{\epsilon_{ikl}}{4e}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{\omega}_k^{(n')} + \tilde{\omega}_k^{(n)}) I_p^{(nn')} I_l^{(nn')} \\ & \qquad + \tfrac{1}{16Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)}) I_p^{(nn')} I_q^{(nn')} I_i^{(nn')} \Big) \\ & = \textstyle\sum_{n'} RCe \Big(I_i^{(nn')} - \tfrac{1}{2Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)}) I_p^{(nn')} I_i^{(nn')} \\ & \qquad + \tfrac{3}{32R^2e^2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)}) I_p^{(nn')} I_q^{(nn')} I_i^{(nn')} \Big). \end{aligned} \tag{3.14}$$

Also, from the second condition of equilibrium, equation (3.9b), we obtain

$$\begin{aligned} & \textstyle\sum_{n'} B\epsilon_{ijk} I_j^{(nn')} \Big(-2ReI_k^{(nn')} + \tilde{u}_k^{(n')} - \tilde{u}_k^{(n)} + \epsilon_{krl} R I_l^{(nn')} (\tilde{\omega}_r^{(n')} + \tilde{\omega}_r^{(n)}) \\ & + \tfrac{1}{2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)}) I_p^{(nn')} I_k^{(nn')} - \tfrac{1}{4Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_k^{(n')} - \tilde{u}_k^{(n)}) I_p^{(nn')} \\ & \qquad - \tfrac{\epsilon_{krl}}{4e}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{\omega}_r^{(n')} + \tilde{\omega}_r^{(n)}) I_p^{(nn')} I_l^{(nn')} \\ & \qquad + \tfrac{1}{16Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)}) I_p^{(nn')} I_q^{(nn')} I_k^{(nn')} \Big) \\ & = \textstyle\sum_{n'} \epsilon_{ijk} RCe I_j^{(nn')} \Big(I_k^{(nn')} - \tfrac{1}{2Re}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)}) I_p^{(nn')} I_k^{(nn')} \\ & \qquad + \tfrac{3}{32R^2e^2}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})(\tilde{u}_q^{(n')} - \tilde{u}_q^{(n)}) I_p^{(nn')} I_q^{(nn')} I_k^{(nn')} \Big). \end{aligned} \tag{3.15}$$

One typical term arising in both of these is $\sum_{n'} I_i^{(nn')}$ and we define

$$J_i^{(n)} = \frac{1}{\eta^{(n)}} \sum_{n'} I_i^{(nn')} \tag{3.16}$$

and also

$$N_{ijk}^{(n)} = \frac{1}{\eta^{(n)}} \sum_{n'} I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} \tag{3.17}$$

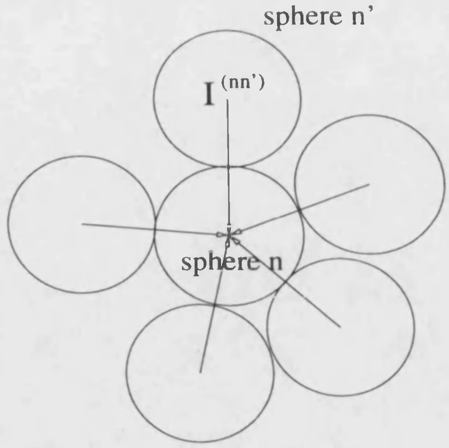

Figure 3-1: *A simple two-dimensional picture of the spheres in contact with the nth*

where $\eta^{(n)}$ is again the number of spheres in contact with the nth. Note that we mentioned $\sum_{n'} I_i^{(nn')}$ earlier in this section and in his work, Walton [86] assumed it to be zero, we now have $\sum_{n'} I_i^{(nn')} = \eta^{(n)} J_i^{(n)}$. This would be zero for an ideal random isotropic packing. A simple two dimensional diagram of a typical sphere, with its contacts and some of the unit vectors which are summed to form $\mathbf{J}^{(n)}$, is shown in figure 3-1 and similarly for $N_{ijk}^{(n)}$.

In order to calculate approximations for $\tilde{u}_i^{(n)}$ and $\tilde{\omega}_i^{(n)}$, we consider the terms of lowest order that arise from equations (3.9). We must make some assumptions concerning the order of particular terms. These assumptions will be non-rigorously justified later. Thus, assuming for now that terms such as $\sum_{n'} \tilde{u}_i^{(n')}$ are of higher order than $\sum_{n'} \tilde{u}_i^{(n)} = \eta^{(n)} \tilde{u}_i^{(n)}$, since we expect the $\tilde{u}_i^{(n')}$ to be uncorrelated, we proceed to find approximations for the perturbations from equations (3.14) and (3.15) above. To start, we consider the lowest order terms arising in this second equation, using our assumptions, these are

$$R(\tilde{\omega}_r^{(n)} \sum_{n'} I_r^{(nn')} I_i^{(nn')} - \eta^{(n)} \tilde{\omega}_i^{(n)}) = 0. \tag{3.18}$$

Now, we require $\sum_{n'} I_r^{(nn')} I_i^{(nn')}$ to first order only since it is multiplied by $\tilde{\omega}_r^{(n)}$. We know that

$$< I_r^{(nn')} I_i^{(nn')} >= \frac{1}{3} \delta_{ir}$$

where the operator $< . >$ represents the average over the sphere surface. Thus, we have

$$\sum_{n'} I_r^{(nn')} I_i^{(nn')} = \frac{\eta^{(n)}}{3}\delta_{ir} + E_{ir}$$

where E_{ir} represents the correction term and so to leading order

$$\sum_{n'} I_r^{(nn')} I_i^{(nn')} = \frac{\eta^{(n)}}{3}\delta_{ir}. \tag{3.19}$$

This allows us to deduce that to first order

$$\tilde{\omega}_i^{(n)} = 0. \tag{3.20}$$

Similarly, the lowest order terms in equation (3.14) are

$$B(-2Re\eta^{(n)}J_i^{(n)} - \eta^{(n)}\tilde{u}_i^{(n)} - \frac{1}{2}\sum_{n'} I_i^{(nn')} I_j^{(nn')} \tilde{u}_j^{(n)}) = RCe(\eta^{(n)}J_i^{(n)} + \frac{3}{4Re}\sum_{n'} I_i^{(nn')} I_j^{(nn')} \tilde{u}_j^{(n)}). \tag{3.21}$$

Using the approximation in equation (3.19) and defining

$$A = \frac{(2B+C)}{(14B+3C)} \tag{3.22}$$

the perturbation $\tilde{u}_i^{(n)}$ to first order, is found to be

$$\tilde{u}_i^{(n)} = -12AReJ_i^{(n)}.$$

Since we require $e < 0$ for compression, then the perturbation $\tilde{u}_i^{(n)}$ is in the same direction as $J_i^{(n)}$. Looking again at figure 3-1, the vector $\mathbf{J}^{(n)}$ is directed towards where there are 'gaps' around the nth sphere. Thus, the perturbation of the displacement is directed towards the gap, which is what we might expect.

We can see that equations (3.8) now give us

$$u_i^{(n)} = e_{ij}X_j^{(n)} - 12AReJ_i^{(n)} \tag{3.23}$$

and

$$\omega_i^{(n)} = 0. \tag{3.24}$$

We look back to our assumption that the order of $\sum_{n'} \tilde{u}_i^{(n')}$ is higher than that of

$\sum_{n'} \tilde{u}_i^{(n)}$. We very roughly justify this by noticing that we would expect a sum over n' of components of the $\mathbf{J}^{(n')}$s, connected with each sphere n', to be uncorrelated and thus some of the elements may cancel. However, a sum over n' of $\mathbf{J}^{(n)}$ 'adds up' to give $\eta^{(n)}\mathbf{J}^{(n)}$.

The expressions found in equation (3.23) and (3.24) can now be substituted back into equation (3.3) to give the following expression, for the force acting on the nth sphere, due to its contact with the n'th:

$$\begin{aligned} F_i^{(nn')} &= \frac{4R^2(-e)^{3/2}}{3\pi B(2B+C)} \Big\{ 2B \Big[I_i + 6A(J_i^{(n')} - J_i^{(n)}) \\ &+3A(J_p^{(n')} - J_p^{(n)})I_pI_i + 18A^2(J_p^{(n')} - J_p^{(n)})(J_i^{(n')} - J_i^{(n)})I_p \\ &\qquad -\frac{9A^2}{2}(J_p^{(n')} - J_p^{(n)})(J_q^{(n')} - J_i^{(n)})I_pI_qI_i \Big] \\ &+C\Big[I_i + \frac{9A}{2}(J_p^{(n')} - J_p^{(n)})I_pI_i \\ &\qquad +\frac{27}{2}(J_p^{(n')} - J_p^{(n)})(J_q^{(n')} - J_q^{(n)})I_pI_qI_i \Big] \Big\} \end{aligned} \tag{3.25}$$

We have omitted the superscripts (nn') on the components of $\mathbf{I}^{(nn')}$ for brevity. We have left in the cross terms such as $J_p^{(n)}J_q^{(n)}$, which although they might appear to be second order in fact reduce to a first order contribution (for details see discussion later in this chapter). We have not included all second order terms only those which turn out to be significant. We checked the other terms but they are of higher order and so we exclude them here so as to avoid undue complexity. The 'second order' terms we have included are needed to ensure consistency for our results when later compared with those from the incremental stage of the problem, upon calculation of the effective moduli.

In the introduction to this chapter we noted that in the numerical simulation results we use for comparison with our theory, the forces occur in chains of particles within the packing. Looking at equation (3.25) with the additional terms, we see that it is possible for the forces to vary within our packing. Considering the two extremes, if $J_i^{(n')}$ and $J^{(n)}$ are in the same direction then they will 'cancel out' in which case the 'J' terms are fairly insignificant in comparison with $\mathbf{I}^{(nn')}$. However, if they are in opposite directions they will 'add up', and it may be possible that both $\mathbf{J}^{(n')}$ and $\mathbf{J}^{(n)}$ are of the order of $\frac{1}{2}\mathbf{I}^{(nn')}$. Taking $\nu = 1/4$, we have $6A \approx 1$, so $6A(\mathbf{J}^{(n')} - \mathbf{J}^{(n)}) \approx \mathbf{I}^{(nn')}$ and then the additional terms make a very significant contribution to the expression. We still do not know whether the largest forces will occur in chains of particles or not, but we at least have the scope for significantly different magnitudes of force acting on different contact areas.

3.2.3 The Average Stress

In this next section we use the equation above, (3.25), to find the average stress within the packing. Previously we introduced the notation $< . >$ to denote

$$< . >= \frac{1}{V} \int_{spheres} . \, dV \tag{3.26}$$

where V is the total volume of the packing. When considering contacts this became equation (1.87), which is the following expression for the average stress within our packing,

$$\begin{aligned} \langle \sigma_{ij} \rangle &= -\frac{R}{V} \sum_{\text{all contacts}} \{ I_i^{(nn')} F_j^{(nn')} + I_j^{(nn')} F_i^{(nn')} \} \\ &= -\frac{3}{8\pi R^2} \frac{1}{N} \sum_n \sum_{n'} \{ I_i^{(nn')} F_j^{(nn')} + I_j^{(nn')} F_i^{(nn')} \} \end{aligned}$$

where V is large and N is the total number of spheres in the packing. What we have actually considered is the limit as $V \to \infty$ or equivalently $N \to \infty$ in which case

$$\langle \sigma_{ij} \rangle = -\frac{3}{8\pi R^2} \lim_{N \to \infty} \frac{1}{N} \sum_n \sum_{n'} \{ I_i^{(nn')} F_j^{(nn')} + I_j^{(nn')} F_i^{(nn')} \}. \tag{3.27}$$

In the limit this sum becomes

$$\langle \sigma_{ij} \rangle = -\frac{3\eta}{8\pi R^2} < I_i F_j + I_j F_i > \tag{3.28}$$

where η is the average co-ordination number within the packing and $< . >$ on the right hand side now represents the average over all directions of the vector $\mathbf{I}^{(nn')}$ or equivalently the integral over the surface of the unit sphere.

Now our expression for the force $\mathbf{F}^{(nn')}$ is not purely a function of $\mathbf{I}^{(nn')}$ and so the definition in this last equation does not hold. However, equation (3.27), does still hold and so we re-define the averaging operator $< . >$ as summing over all contacts, that is over both spheres n and n'. N is the total number of spheres within the total volume

V and η is the average co-ordination number again. With $< . >$ re-defined we have

$$\langle \sigma_{ij} \rangle = -\frac{R\eta N}{2V} < I_i^{(nn')} F_j^{(nn')} + I_j^{(nn')} F_i^{(nn')} > . \tag{3.29}$$

We define the following typical packing parameters that arise in the calculation of this stress:

$$\begin{aligned} \alpha_{ij} &= \langle I_i^{(nn')} J_j^{(n)} \rangle \\ \beta_{ijkl} &= \langle I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} J_l^{(n)} \rangle \\ \gamma_{ijkl} &= \langle I_i^{(nn')} I_j^{(nn')} J_k^{(n)} J_l^{(n)} \rangle \\ \zeta_{ijklmn} &= \langle I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} I_l^{(nn')} I_m^{(nn')} J_n^{(n)} \rangle \\ \eta_{ijklmn} &= \langle I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} I_l^{(nn')} J_m^{(n)} J_n^{(n)} \rangle . \end{aligned} \tag{3.30}$$

We start by considering α_{ij}, we expect it to be small and isotropic as there is no preferred direction for $I_i^{(nn')}$ or $J_i^{(n)}$. Thus, let

$$\alpha_{ij} = \alpha \delta_{ij}.$$

In two dimensions it is possible to find α analytically for some co-ordination numbers (see Chapter 4). However, in three dimensions, as we are concerned with, the question arises as to how to order the spheres and so analytical methods become extremely difficult. The value of α is calculated using computer simulation instead. Its value decreases with increasing co-ordination number. In order to calculate a value for α, we notice that

$$\alpha = \frac{1}{3} < I_i^{(nn')} J_i^{(n)} > = \frac{1}{3N\eta} \sum_n \sum_{n'} I_i^{(nn')} J_i^{(n)} = \frac{1}{3N\eta} \sum_n \eta^{(n)} J_i^{(n)} J_i^{(n)}, \tag{3.31}$$

where summing is over n', the spheres in contact with the nth, and n all the spheres in the packing. The calculations for both two and three dimensional problems are discussed in more detail in Chapter 4.

In a random packing the tensors in equations (3.30) are isotropic and satisfy certain symmetries. β_{ijkl} is a fourth order isotropic tensor which must be symmetric if we interchange any two of i, j and k. Any fourth order isotropic tensor is a linear combination of $\delta_{ij}\delta_{kl}$, $\delta_{ik}\delta_{jl}$ and $\delta_{il}\delta_{jk}$. To satisfy the above symmetries the only combination we can have is:

$$\beta_{ijkl} = \beta(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{3.32}$$

However, since $I_p^{(nn')} I_p^{(nn')} = 1$ if we let $j = k$ in equation (3.30b) then

$$\begin{aligned}
\beta_{ikkl} &= < I_i^{(nn')} I_k^{(nn')} I_k^{(nn')} J_l^{(n)} > \\
&= < I_i^{(nn')} J_l^{(n)} > \\
&= \alpha_{il} \\
&= \alpha\delta_{il}.
\end{aligned}$$

Now from equation (3.32) we have

$$\beta_{ikkl} = 5\beta\delta_{il}$$

so then $\beta = \alpha/5$ and hence

$$\beta_{ijkl} = \frac{\alpha}{5}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{3.33}$$

Now, γ_{ijkl} is also a fourth order isotropic tensor and it should be symmetric if we interchange i and j or k and l. The only combination which satisfies this is

$$\gamma_{ijkl} = \gamma_1\delta_{ij}\delta_{kl} + \gamma_2(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{3.34}$$

To determine γ_1 and γ_2 this time we consider the definition of the averaging operator which is the sum over all contacts. We can rewrite the expression for α_{ij} as given in equation (3.31), in terms of sums as follows:

$$\alpha_{ij} = \frac{1}{3N\eta}\sum_n\sum_{n'} I_i^{(nn')} J_j^{(n)} \tag{3.35}$$

and so similarly

$$\begin{aligned}
\gamma_{ijkl} &= \frac{1}{3N\eta}\sum_n\sum_{n'} I_i^{(nn')} I_j^{(nn')} J_k^{(n)} J_l^{(n)} \\
&= \frac{1}{3N\eta}\sum_n J_k^{(n)} J_l^{(n)} \sum_{n'} I_i^{(nn')} I_j^{(nn')}.
\end{aligned} \tag{3.36}$$

We wish to find $\sum_{n'} I_i^{(nn')} I_j^{(nn')}$ to leading order since it is multiplied by $J_k^{(n)} J_l^{(n)}$. Now

$$< I_i^{(nn')} I_j^{(nn')} >= \frac{1}{3}\delta_{ij}$$

and so we approximate $\sum_{n'} I_i^{(nn')} I_j^{(nn')}$ by

$$\sum_{n'} I_i^{(nn')} I_j^{(nn')} \approx \frac{\eta^{(n)}}{3}\delta_{ij}.$$

Thus to first order we have

$$\begin{aligned} \gamma_{ijkl} &= \frac{1}{9N\eta}\delta_{ij}\sum_n J_k^{(n)} J_l^{(n)} \\ &= \frac{\alpha}{3}\delta_{ij}\delta_{kl}. \end{aligned}$$

Now in equation (3.34) we have $\gamma_1 = \alpha/3$ and $\gamma_2 = 0$ and so, to leading order,

$$\gamma_{ijkl} = \frac{\alpha}{3}\delta_{ij}\delta_{kl}. \tag{3.37}$$

Both ζ_{ijklmn} and η_{ijklmn} are sixth order isotropic tensors and so are linear combinations of fifteen terms such as $\delta_{ij}\delta_{kl}\delta_{mn}$. In particular, we want ζ_{ijklmn} to be symmetric upon interchange of any two from i, j, k, l, and m. The only combination that satisfies this is

$$\begin{aligned} \zeta_{ijklmn} = \; & \zeta\left(\delta_{ij}(\delta_{kl}\delta_{mn} + \delta_{km}\delta_{ln} + \delta_{kn}\delta_{lm}) + \delta_{ik}(\delta_{jl}\delta_{mn} + \delta_{jm}\delta_{ln} + \delta_{jn}\delta_{lm})\right. \\ & + \delta_{il}(\delta_{jk}\delta_{mn} + \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km}) + \delta_{im}(\delta_{jk}\delta_{ln} + \delta_{jl}\delta_{kn} + \delta_{jn}\delta_{kl}) \\ & \left. + \delta_{in}(\delta_{jk}\delta_{lm} + \delta_{jl}\delta_{km} + \delta_{jm}\delta_{kl})\right). \end{aligned} \tag{3.38}$$

Again, using the fact that $I_p^{(nn')} I_p^{(nn')} = 1$ and the same method that was used to determine β_{ijkl} above we find

$$\begin{aligned} \zeta_{ijklmn} = \; & \frac{\alpha}{35}\left(\delta_{ij}(\delta_{kl}\delta_{mn} + \delta_{km}\delta_{ln} + \delta_{kn}\delta_{lm}) + \delta_{ik}(\delta_{jl}\delta_{mn} + \delta_{jm}\delta_{ln} + \delta_{jn}\delta_{lm})\right. \\ & + \delta_{il}(\delta_{jk}\delta_{mn} + \delta_{jm}\delta_{kn} + \delta_{jn}\delta_{km}) + \delta_{im}(\delta_{jk}\delta_{ln} + \delta_{jl}\delta_{kn} + \delta_{jn}\delta_{kl}) \\ & \left. + \delta_{in}(\delta_{jk}\delta_{lm} + \delta_{jl}\delta_{km} + \delta_{jm}\delta_{kl})\right). \end{aligned} \tag{3.39}$$

This just leaves η_{ijklmn} which must be symmetric upon interchange of any two of i, j,

k and l and also upon interchange of m and n. Hence it must be represented as follows:

$$\begin{aligned}\eta_{ijklmn} &= \eta_1\delta_{ij}(\delta_{kl}\delta_{mn}+\delta_{km}\delta_{ln}+\delta_{kn}\delta_{lm})) \\ &\quad +\eta_2\left(\delta_{ik}(\delta_{jl}\delta_{mn}+\delta_{jm}\delta_{ln}+\delta_{jn}\delta_{lm})+\delta_{il}(\delta_{jk}\delta_{mn}+\delta_{jm}\delta_{kn}+\delta_{jn}\delta_{km})\right. \\ &\quad \left.+\delta_{im}(\delta_{jk}\delta_{ln}+\delta_{jl}\delta_{kn}+\delta_{jn}\delta_{kl})+\delta_{in}(\delta_{jk}\delta_{lm}+\delta_{jl}\delta_{km}+\delta_{jm}\delta_{kl})\right). \quad (3.40)\end{aligned}$$

The same method that we used to find γ_{ijkl} enables us to calculate

$$\eta_{ijklmn} = \frac{\alpha}{15}\delta_{mn}\left(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{jk}\delta_{il}\right),$$

but this time using the approximation $\sum_{n'} I_i^{(nn')}I_j^{(nn')}I_k^{(nn')}I_l^{(nn')} = \frac{\eta^{(n)}}{15}(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})$.

At this point, we also define the parameter χ:

$$\chi = \frac{1}{3} < N_{ijk}^{(n)} I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} > \quad (3.41)$$

which is not actually required in this stage of the problem, but will be needed in the next section, when we consider the application of an additional incremental deformation, to the boundary of the packing.

Returning to calculation of the average stress, we must also consider some of the properties of the averaging operator. Considering first the n'th sphere it can be seen, from equation (3.4), that

$$\langle I_i^{(nn')} J_j^{(n')}\rangle = -\langle I_i^{(n'n)} J_j^{(n')}\rangle$$

and since

$$\langle I_i^{(n'n)} J_j^{(n')}\rangle = \langle I_i^{(nn')} J_j^{(n)}\rangle$$

then

$$\langle I_i^{(nn')} J_j^{(n')}\rangle = -\langle I_i^{(nn')} J_j^{(n)}\rangle. \quad (3.42)$$

Our aim is to find $\langle\sigma_{ij}\rangle$ and we need all these results along with two that we have seen earlier. These are

$$\langle I_i^{(nn')} I_j^{(nn')}\rangle = \frac{1}{3}\delta_{ij},$$

$$\langle I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} I_l^{(nn')} \rangle = \frac{1}{15}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \tag{3.43}$$

Having substituted for $\mathbf{F}^{(nn')}$ into equation (3.29) and using all the results above then after some manipulation, the expression for the average stress reduces to:

$$\langle \sigma_{ij} \rangle = -\frac{\phi\eta(-e)^{3/2}}{3\pi^2 B}\{1 - 27A(2-A)\alpha\}\delta_{ij} \tag{3.44}$$

where ϕ is again the volume concentration of the spheres, first met in Chapter 1 and given by

$$\phi = \frac{4\pi R^3 N}{3V}. \tag{3.45}$$

We note the extra terms introduced by our perturbation when compared with Walton's [86] expression for the average stress, found using the uniform strain approximation:

$$< \sigma_{ij} >= -\frac{\phi\eta(-e)^{3/2}}{3\pi^2 B}. \tag{3.46}$$

This was previously seen in Chapter 1, equations (1.94) and (1.95).

All of the above results apply for spheres that are infinitely rough. We now consider the case when they are perfectly smooth, following the same methods used above. The general expression for the force acting on the nth sphere due to its contact with the n'th is now given by:

$$\mathbf{F}^{(nn')} = \frac{(2R)^{1/2}}{3\pi B}[(\mathbf{u}_i^{(n')} - \mathbf{u}_i^{(n)}).\mathbf{I}^{(nn')}]^{3/2}\mathbf{I}^{(nn')}. \tag{3.47}$$

We assume that after the initial hydrostatic compression has been applied to the boundary, the displacement of the centre of the nth sphere is given by:

$$u_i^{(n)} = e_{ij}X_j^{(n)} + \tilde{u}_i^{(n)}$$

and

$$\omega_i^{(n)} = \tilde{\omega}_i^{(n)}.$$

Again, considering equilibrium of forces and moments acting on the nth sphere allows us to calculate the perturbations, $\tilde{u}_i^{(n)}$ and $\tilde{\omega}_i^{(n)}$, to leading order. These are given by

$$\tilde{u}_i^{(n)} = -4ReJ_i^{(n)}$$

and

$$\tilde{\omega}_i^{(n)} = 0.$$

Hence

$$\begin{aligned} F_i^{(nn')} &= \frac{4R^2(-e)^{3/2}}{3\pi B}\left\{I_i^{(nn')} + 3(J_p^{(n')} - J_p^{(n)})I_p^{(nn')}I_i^{(nn')}\right. \\ &\quad \left. + \frac{3}{2}(J_p^{(n')} - J_p^{(n)})(J_q^{(n')} - J_q^{(n)})I_p^{(nn')}I_q^{(nn')}I_i^{(nn')}\right\} \end{aligned} \tag{3.48}$$

and from this, using the parameters defined above, we find the average stress to be

$$\langle \sigma_{ij} \rangle = -\frac{\phi\eta(-e)^{3/2}}{3\pi^2 B}\left\{1 - 15\alpha\right\}. \tag{3.49}$$

As we would expect, this is consistent with the expression derived from taking the limit $\frac{C}{B} \to \infty$ in equation (3.44).

For completeness, we should also consider the case when we impose an initial uniaxial compression upon our random packing of spheres. However, the calculations are not so manageable. The strain now has the form

$$e_{ij} = e_3\delta_{i3}\delta_{j3}$$

and we again let the displacement of the centre of the nth sphere after the initial deformation be $u_i^{(n)} = e_{ij}X_j^{(n)} + \tilde{u}_i^{(n)}$ and $\omega_i^{(n)} = \Omega_i + \tilde{\omega}_i^{(n)} = \tilde{\omega}_i^{(n)}$. We find the expression for the force acting on the nth sphere due to its contact with the n'th is:

$$\begin{aligned} F_i^{(nn')} &= \frac{2R(-e_3)^{1/2}}{3\pi B(2B+C)}\left[|I_3^{(nn')}| - (\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})\frac{I_p^{(nn')}}{4Re_3|I_3^{(nn')}|}\right]\left\{2B\left(-2Re_3\delta_{i3}I_3^{(nn')}\right.\right. \\ &\quad \left. + (\tilde{u}_i^{(n')} - \tilde{u}_i^{(n)}) + \epsilon_{ikl}RI_l^{(nn')}(\omega_k^{(n')} + \omega_k^{(n)})\right) \\ &\quad \left. + 2RC(-e_3)[(I_3^{(nn')})^2 - \frac{1}{2Re_3}(\tilde{u}_p^{(n')} - \tilde{u}_p^{(n)})I_p^{(nn')}]I_i^{(nn')}\right\}. \end{aligned} \tag{3.50}$$

Now, using the equilibrium of moments and forces we obtain first order approximations for $\tilde{u}_i^{(n)}$ and $\tilde{\omega}_i^{(n)}$. If $i = 1$ or $i = 2$:

$$\tilde{u}_i^{(n)} = -\frac{32Re_3C\sum_{n'}|I_3^{(nn')}|(I_3^{(nn')})^2 I_i^{(nn')}}{\eta^{(n)}(16B+3C)},$$

and when $i = 3$

$$\tilde{u}_3^{(n)} = -\frac{16Re_3(2B\sum_{n'}|I_3^{(nn')}|I_3^{(nn')} + C\sum_{n'}|I_3^{(nn')}|(I_3^{(nn')})^3)}{3\eta^{(n)}(4B+3C)}$$

where $\eta^{(n)}$ is the co-ordination number of the nth sphere. For any value of i,

$$\tilde{\omega}_i^{(n)} = 0.$$

From these we could continue by substituting back into the force expression and then calculate the average stress, proceeding by the same method discussed above for an initial hydrostatic compression. However, the algebra becomes extremely messy and involves many more unknown parameters and so we have not pursued this any further.

In the case of a biaxial strain, it would also be possible to work out the effective moduli when the strain takes the form:

$$e_{ij} = e\delta_{ij} + \Delta e_3\delta_{i3}\delta_{j3}. \tag{3.51}$$

However, the algebra becomes even more cumbersome and messy than in the uniaxial case, so although some attempts were made to start upon this calculation, they were abandoned.

3.2.4 The Effective Moduli

To calculate the effective moduli, we suppose that our packing is now subject to a further incremental deformation. The boundary of the packing will undergo a further displacement

$$\delta u_i = \delta e_{ij}x_j. \tag{3.52}$$

Walton's work [86] again assumes that under this compression the centre of the nth will be displaced in accordance with the uniform strain approximation. We modify this approximation and then the centre of the nth sphere is displaced by $\delta u_i^{(n)}$ and $\delta\omega_i^{(n)}$ where

$$\delta u_i^{(n)} = \delta e_{ij}X_j^{(n)} + \delta\tilde{u}_i^{(n)} \tag{3.53}$$

and

$$\delta\omega_i^{(n)} = \delta\Omega_i + \delta\tilde{\omega}_i^{(n)}. \tag{3.54}$$

In a packing of infinitely rough spheres, the incremental force on the nth sphere due to its contact with the n'th sphere is given by equation (1.141) as

$$\begin{aligned}\delta F_i^{(nn')} &= \frac{(2R)^{1/2}}{2\pi B(2B+C)}[(u_p^{(n')}-u_p^{(n)})I_p^{(nn')}]^{1/2}\left\{2B(\delta u_i^{(n')}-\delta u_i^{(n)}+\right.\\ &\left. R\epsilon_{ijk}(\delta\omega_j^{(n')}+\delta\omega_j^{(n)})I_k^{(nn')})+C[(\delta u_p^{(n')}-\delta u_p^{(n)})I_p^{(nn')}]I_i^{(nn')}\right\}. \quad (3.55)\end{aligned}$$

To calculate further an expression for this force, we must find approximations for $\delta\tilde{u}_i^{(n)}$ and $\delta\tilde{\omega}_i^{(n)}$. In order to do this, we initially consider just the first order terms of the equations of equilibrium, in the same way as we did in the initial part of the problem, equations (3.18) and (3.21). We have

$$\begin{aligned}\sum_{n'}\delta F_i^{(nn')} &= 0,\\ \sum_{n'}\epsilon_{ijk}I_j^{(nn')}\delta F_k^{(nn')} &= 0. \end{aligned} \quad (3.56)$$

These yield two equations similar to (3.14) and (3.15) and in order to find first order approximations for $\delta\tilde{u}_i^{(n)}$ and $\delta\tilde{\omega}_i^{(n)}$, we must discard some of the terms and we make the same kind of assumptions which led to equations (3.18) and (3.21). From these we find that to first order,

$$\begin{aligned}\delta\tilde{u}_i^{(n)} &= -\frac{6R}{(6B+C)}[2B(1-A)\delta e_{ik}J_k^{(n)}\\ &\qquad +C\delta e_{kl}(N_{ikl}^{(n)}-3AV_{iklm}^{(n)}J_m^{(n)})] \end{aligned} \quad (3.57)$$

and

$$\delta\tilde{\omega}_i^{(n)} = 0. \quad (3.58)$$

The term $V_{ijkl}^{(n)}$ is defined by

$$V_{ijkl}^{(n)} = \frac{\sum_{n'} I_i^{(nn')}I_j^{(nn')}I_k^{(nn')}I_l^{(nn')}}{\eta^{(n)}} \quad (3.59)$$

and since it is multiplied by $J_m^{(n)}$, we need only approximate it to leading order. Since

$$< I_i^{(nn')}I_j^{(nn')}I_k^{(nn')}I_l^{(nn')} >= \frac{1}{15}(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})$$

then we use the following approximation for $V_{ijkl}^{(n)}$,

$$V_{ijkl}^{(n)} = \frac{1}{15}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}). \qquad (3.60)$$

The terms $J_k^{(n)}$ and $N_{ikl}^{(n)}$ are previously defined in equations (3.16) and (3.17).

Substituting equations (3.57) and (3.58) back into equation (3.55), we can now find $\delta F_i^{(nn')}$, to leading order, which is given by the following lengthy expression:

$$\begin{aligned}
\delta F_i^{(nn')} = & -\frac{4R^2(-e)^{1/2}}{2\pi B(2B+C)}\Big\{2B\Big[\delta e_{ip}I_p + \frac{3}{(6B+C)}\Big(2B(1-A)\delta e_{ip}(J_p^{(n')} - J_p^{(n)}) \\
& +C\delta e_{pq}(N_{ipq}^{(n')} - N_{ipq}^{(n)} - 3A(V_{ipqm}^{(n')}J_m^{(n')} - V_{ipqm}^{(n)}J_m^{(n)}))\Big) + 3A\delta e_{iq}((J_p^{(n')} - J_p^{(n)})I_qI_p \\
& +\frac{9A}{(6B+C)}\Big(2B(1-A)\delta e_{ip}(J_p^{(n')} - J_p^{(n)}) + C\delta e_{pq}(N_{ipq}^{(n')} - N_{ipq}^{(n)} \\
& \qquad -3A(V_{ipqm}^{(n')}J_m^{(n')} - V_{ipqm}^{(n)}J_m^{(n)})\Big)(J_s^{(n')} - J_s^{(n)})I_s \\
& \qquad -\frac{9}{2}A^2R\delta e_{ip}(J_m^{(n')} - J_m^{(n)})(J_q^{(n')} - J_q^{(n)})I_pI_mI_q\Big] \\
& +C\Big[\delta e_{pq}I_pI_qI_i + \frac{3}{(6B+C)}\Big(2B(1-A)\delta e_{sp}(J_p^{(n')} - J_p^{(n)}) \\
& \qquad +C\delta e_{pq}(N_{spq}^{(n')} - N_{spq}^{(n)} - 3A(V_{spqm}^{(n')}J_m^{(n')} - V_{spqm}^{(n)}J_m^{(n)}))\Big)I_sI_i \\
& +3A\delta e_{pq}I_pI_qI_iI_m(J_m^{(n')} - J_m^{(n)}) + \frac{9A}{(6B+C)}\Big(2B(1-A)\delta e_{sp}(J_p^{(n')} - J_p^{(n)}) \\
& +C\delta e_{pq}(N_{spq}^{(n')} - N_{spq}^{(n)} - 3A(V_{spqm}^{(n')}J_m^{(n')} - V_{spqm}^{(n)}J_m^{(n)})\Big)(J_t^{(n')} - J_t^{(n)})I_sI_tI_i \\
& \qquad -\frac{9}{2}A^2R\delta e_{pq}I_p(J_m^{(n')} - J_m^{(n)})(J_t^{(n')} - J_t^{(n)})I_mI_tI_pI_qI_i\Big]\Big\}. \qquad (3.61)
\end{aligned}$$

Since this expression is long, we have omitted the superscripts (nn') from the components of $\mathbf{I}^{(nn')}$, to keep it as concise as possible.

From this we proceed to substitute into the following equation to find average the incremental stress,

$$\langle\delta\sigma_{ij}\rangle = -\frac{R\eta N}{2V}\langle I_i^{(nn')}\delta F_j^{(nn')} + I_j^{(nn')}\delta F_i^{(nn')}\rangle. \qquad (3.62)$$

The terms that arise are similar to those in section 3.2.3 and after some manipulation we have

$$\begin{aligned}
\langle\delta\sigma_{ij}\rangle = & \frac{3\phi\eta(-e)^{1/2}}{2\pi^2B(2B+C)}\Big\{B\Big[\frac{1}{3}(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - \frac{12(1-A)\alpha}{(14B+3C)}\Big((2B + \frac{2C}{5})(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\
& +\frac{2C}{5}\delta_{ij}\delta_{kl}\Big) - 3A\alpha(2+A)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\Big] + C\Big[\frac{1}{15}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})
\end{aligned}$$

$$-\frac{6}{(6B+C)}\Bigg(\frac{2B(1-A)\alpha}{5}(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})+C(\frac{1}{5}(2\alpha-\chi)\delta_{ij}\delta_{kl}$$
$$+\frac{1}{10}(3\chi-\alpha)(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})-\frac{A\alpha}{25}(7\delta_{ij}\delta_{kl}+2(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))\Bigg)$$
$$-\frac{6A\alpha}{5}(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})+\frac{12A\alpha}{5(14B+3C)}\Bigg((2B+\frac{7C}{5})\delta_{ij}\delta_{kl}$$
$$+(2B+\frac{2C}{5})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\Bigg)-\frac{3A^2\alpha}{5}(\delta_{ij}\delta_{kl}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\Bigg]\Bigg\}\,\delta e_{kl}, \tag{3.63}$$

where α and χ are defined in equations (3.30) and (3.41) respectively. In general, the average incremental stress is related to the average incremental strain, $\langle\delta e_{ij}\rangle$ as follows,

$$\langle\delta\sigma_{ij}\rangle = C^*_{ijkl}\langle\delta e_{ij}\rangle. \tag{3.64}$$

For an initial hydrostatic compression, we know that

$$C^*_{ijkl} = \lambda^*\delta_{ij}\delta_{kl}+\mu^*(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}), \tag{3.65}$$

and thus we can calculate the effective moduli in this case. Hence, we have

$$\begin{aligned}\lambda^* \;=\; & \frac{\phi\eta C(-e)^{1/2}}{10\pi^2B(2B+C)}\left\{1-9A(2+A)\alpha-\frac{72(1-A)B}{(14B+3C)}\alpha\right.\\ & \left.+\frac{36(1-A)(10B+7C)}{5(14B+3C)}\alpha-\frac{18C}{(6B+C)}\left(\frac{3}{5}\alpha-\chi\right)\right\}\end{aligned} \tag{3.66}$$

and

$$\begin{aligned}\mu^* \;=\; & \frac{\phi\eta(5B+C)(-e)^{1/2}}{10\pi^2B(2B+C)}\left\{1-9A(2+A)\alpha-\frac{72(1-A)(5B+C)}{5(14B+3C)}\alpha\right.\\ & \left.-\frac{54C^2}{10(6B+C)(5B+C)}(5\chi-3\alpha)\right\},\end{aligned} \tag{3.67}$$

where ϕ is as given in equation (3.45). These are the main new results for this chapter, they give the modified expressions for the effective Lamé moduli of a random packing of equal sized spheres, upon application of an initial hydrostatic compression.

We can also calculate the effective bulk modulus, for comparison with the results of Jenkins *et al.* [43],

$$\kappa^* = \lambda^* + \frac{2}{3}\mu^*$$

and so

$$\kappa^* = \frac{\phi\eta(-e)^{1/2}}{6\pi^2 B}\left\{1 - 27A(2-A)\alpha\right\}. \tag{3.68}$$

This is clearly consistent with the expression we found for the average initial stress in equation (3.44), which yields the same expression for the bulk modulus upon differentiation.

The expressions found for these moduli by Walton [86] are,

$$\begin{aligned} \lambda^* &= \frac{\phi\eta C(-e)^{1/2}}{10\pi^2 B(2B+C)}, \\ \mu^* &= \frac{\phi\eta(5B+C)(-e)^{1/2}}{10\pi^2 B(2B+C)} \end{aligned} \tag{3.69}$$

and

$$\kappa^* = \frac{\phi\eta(-e)^{1/2}}{6\pi^2 B} \tag{3.70}$$

and so we can easily note the extra terms that occur in our new expressions. Assuming $\mathbf{J}^{(n)}$ to be zero as did Walton [86], then $\alpha = \chi = 0$ and we see that our results are identical to these.

These results apply only when the spheres are infinitely rough. For the case of perfectly smooth spheres the force acting on the nth sphere due to its contact with the n'th is

$$\delta\mathbf{F}^{(nn')} = \frac{(2R)^{1/2}}{2\pi B}\left\{[(\mathbf{u}^{(n')} - \mathbf{u}^{(n)}).\mathbf{I}^{(nn')}]^{1/2}((\delta\mathbf{u}^{(n')} - \delta\mathbf{u}^{(n)}).\mathbf{I}^{(nn')})\right\}\mathbf{I}^{(nn')}. \tag{3.71}$$

If the displacement of the sphere centre is again given by a perturbation of the uniform strain approximation then

$$\delta u_i^{(n)} = \delta e_{ij} X_j^{(n)} + \delta\tilde{u}_i^{(n)}$$

and

$$\delta\omega_i^{(n)} = \delta\Omega_i + \delta\tilde{\omega}_i^{(n)}.$$

Considering the equations of equilibrium to first order allows us to calculate

$$\delta u_i^{(n)} = \delta e_{ij} X_j^{(n)} - 6R\delta e_{pq}(N_{ipq}^{(n)} - J_s^{(n)} V_{ipqs}^{(n)}) \tag{3.72}$$

and

$$\delta\omega_i^{(n)} = 0. \tag{3.73}$$

Using this in turn, we find the incremental force to first order. We have

$$\begin{aligned}\delta F_i^{(nn')} &= -\frac{2R^2(-e)^{1/2}}{\pi B}\Big\{\delta e_{rs}I_rI_sI_i + 3[\delta e_{pr}(N_{prs}^{(n')} - N_{prs}^{(n)} - (J_q^{(n')}V_{pqrs}^{(n')} - J_q^{(n)}V_{pqrs}^{(n)}))]I_sI_i \\ &\qquad + \delta e_{rs}(J_p^{(n')} - J_p^{(n)})I_pI_rI_sI_i \\ &\quad + 3[\delta e_{pr}(N_{prs}^{(n')} - N_{prs}^{(n)} - (J_q^{(n')}V_{pqrs}^{(n')} - J_q^{(n)}V_{pqrs}^{(n)}))](J_m^{(n')} - J_m^{(n)})I_mI_sI_i \\ &\qquad -\frac{1}{2}\delta e_{rs}(J_p^{(n')} - J_p^{(n)})(J_q^{(n')} - J_q^{(n)})I_pI_qI_rI_sI_i \\ &- \frac{3}{2}[\delta e_{pr}(N_{prs}^{(n')} - N_{prs}^{(n)} - (J_q^{(n')}V_{pqrs}^{(n')} - J_q^{(n)}V_{pqrs}^{(n)}))](J_m^{(n')} - J_m^{(n)})(J_v^{(n')} - J_v^{(n)})I_mI_vI_sI_i\Big\},\end{aligned} \tag{3.74}$$

where the superscripts (nn') on the components of $\mathbf{I}^{(nn')}$, have again been omitted for brevity.

The average incremental stress follows from this, through equation (3.62) and is found to be

$$\begin{aligned}\langle\delta\sigma_{ij}\rangle &= \frac{\phi\eta(-e)^{1/2}}{10\pi^2 B}\{(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) - (29\delta_{ij}\delta_{kl} + 6(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}))\alpha \\ &\qquad + 9(2\delta_{ij}\delta_{kl} - 3(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}))\chi\}.\end{aligned} \tag{3.75}$$

The effective moduli are then calculated as

$$\begin{aligned}\lambda^* &= \frac{\phi\eta(-e)^{1/2}}{10\pi^2 B}(1 - 29\alpha + 18\chi) \\ \mu^* &= \frac{\phi\eta(-e)^{1/2}}{10\pi^2 B}(1 + 6\alpha - 27\chi).\end{aligned} \tag{3.76}$$

To calculate the effective bulk modulus we again use $\kappa^* = \lambda^* + \frac{2}{3}\mu^*$, this gives

$$\kappa^* = \frac{\phi\eta(-e)^{1/2}}{6\pi^2 B}\{1 - 15\alpha\}. \tag{3.77}$$

Walton's results for the effective moduli of a packing of perfectly smooth spheres are

$$\lambda^* = \mu^* = \frac{\phi\eta(-e)^{1/2}}{10\pi^2 B}$$

and

$$\kappa^* = \frac{\phi\eta(-e)^{1/2}}{6\pi^2 B}$$

and our results are again clearly consistent with these, when $\alpha = \chi = 0$.

Poisson's ratio can also be calculated for the two cases of friction considered. It is defined by:

$$\nu^* = \frac{\lambda^*}{2(\lambda^* + \mu^*)} \tag{3.78}$$

and for the case of infinitely rough spheres is

$$\nu^* = \frac{\nu\left\{(14-11\nu)^2 + 9(17\nu^2 - 292\nu + 324)\alpha - \frac{18(14-11\nu)^2}{(6-5\nu)}\left(\frac{3}{5}\alpha - \chi\right)\right\}}{2\left\{(5-3\nu)((14-11\nu)^2 - 18(9\nu^3 - 271\nu^2 - 520\nu - 252)\alpha) - \frac{18\nu(14-11\nu)^2}{(6-5\nu)}\left((15-13\nu)\chi - \frac{3}{10}(15-14\nu)\alpha\right)\right\}}. \tag{3.79}$$

When $\alpha = \chi = 0$, we recover the result for Poisson's ratio found by Walton [86], as we would expect.

For a packing of perfectly smooth spheres Poisson's ratio is given by

$$\nu^* = \frac{1 - 29\alpha + 18\chi}{2(2 - 23\alpha - 9\chi)} \tag{3.80}$$

and this reduces to 1/4 when $\alpha = \chi = 0$ as deduced by Walton [86].

In the next chapter, we describe the simulations which enabled us to estimate values of the unknown parameters α and χ which occur in the modified expressions for the effective elastic moduli of the sphere packing. Using these, we were able to obtain revised predictions for the values of the moduli for comparison with the work of Jenkins *et al.* [43].

Chapter 4

Numerical Calculation of α and χ Terms

This chapter deals with the calculation of numerical values for the parameters α and χ that occur in the equal sized sphere packings described in Chapter 3. In order to compare our new theory with the numerical simulation results of Jenkins *et al.* [43] we must estimate the change to the numerical values predicted for the effective elastic moduli, caused by these unknown parameters.

For the specific results we require, the parameters were determined by computer simulation. In this chapter however, we also consider analytical calculations, some work is done in both two and three dimensions. To be physically realistic we require that each sphere be in equilibrium, however for completeness we also consider collections of spheres that are not in equilibrium.

4.1 A Packing of Equal Sized Spheres

Using just a first order perturbation of the uniform strain approximation, on a packing of equal sized spheres, we have to consider two parameters which arise in the calculations. These are α and χ, as previously defined in Chapter 3 by

$$\alpha = \frac{1}{3} < I_i^{(nn')} J_i^{(n)} >$$

and

$$\chi = \frac{1}{3} < I_i^{(nn')} I_j^{(nn')} I_k^{(nn')} N_{ijk}^{(n)} >$$

where $I_i^{(nn')}$ is the unit vector along the line of centres between the nth and n'th spheres and

$$J_i^{(n)} = \frac{1}{\eta^{(n)}} \sum_{n'} I_i^{(nn')}$$

and

$$N_{ijk}^{(n)} = \frac{1}{\eta^{(n)}} \sum_{n'} I_i^{(nn')} I_j^{(nn')} I_k^{(nn')}.$$

The averaging operator $< . >$ represents the average over all contacts within the packing and the sum over n' is that over all spheres in contact with the nth. The operator $< . >$ is thus equivalent to summing over both n and n'. Both α and χ represent a measure of how much the behaviour of the packing deviates from that of an ideal random packing. If the behaviour were ideal then $\alpha = \chi = 0$ and we would have recovered Walton's results [86].

For our purposes it is easier to re-write α and χ as

$$\alpha = \frac{1}{3N\eta} \sum_n \eta^{(n)} J_i^{(n)} J_i^{(n)} \tag{4.1}$$

and

$$\chi = \frac{1}{3N\eta} \sum_n \eta^{(n)} N_{ijk}^{(n)} N_{ijk}^{(n)} \tag{4.2}$$

where N is the total number of spheres in the packing, $\eta^{(n)}$ is the co-ordination number of the nth sphere, η is the average co-ordination number and the sum is taken over all spheres n in the packing.

In two dimensions, it is simple to calculate by hand a value for α. Considering spheres in contact with the nth sphere, these can be ordered and it is easy to 'visualise' the situation. However, in 3-D it is much more difficult to visualise. The question arises as to how to order the spheres. In this case we turn to computer simulation to help us calculate the expected value. In the next section we start by considering the expected value of the parameter α, for a random arrangement of discs in 2-D.

4.1.1 Analytical Methods and Simulation in 2-D

In 2-D, it is possible to calculate the expected value of α analytically and these values could then also be confirmed using computer simulation, if required. Even though these results were not used in the calculation of values for the new effective moduli, they were

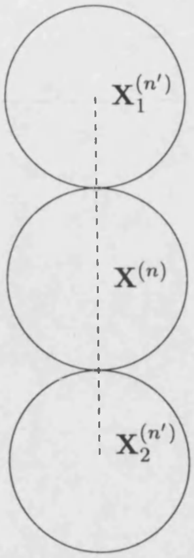

Figure 4-1: *Condition for equilibrium of the nth disc in contact with just two others*

carried out in order to build up a more complete picture about what influences the value of each parameter. We consider, for example, the effect of increasing or decreasing co-ordination number, noting any trend in the values. We would expect to find similar patterns when we later consider the 3-D case.

We are primarily concerned with equilibrium of each disc. However, we shall look at both the restricted case of each disc in equilibrium and also any general arrangement of contacting discs. In particular, we require equilibrium of the nth disc, say. In 2-D, we will need a minimum of four discs in contact with the nth such that any combination we choose ensures equilibrium of the nth disc. If we have just three discs in contact with the nth then some combinations will be in equilibrium while others will not. We shall only consider values of the parameter α at this stage.

Starting with just one disc in contact with the nth it is impossible to attain equilibrium, but we can still calculate that in this case $|J^{(n)}|^2 = 1$ and so α=1/3.

With two discs in contact with the nth it is generally not possible to have equilibrium. The unique case when there is equilibrium arises when the two discs are on exactly opposite sides of the nth, see figure 4-1. In this special case the value of $\mathbf{J}^{(n)}$ is $\mathbf{0}$ and so $\alpha = 0$.

Now, we consider any two discs in contact with the nth, see figure 4-2. We pick our

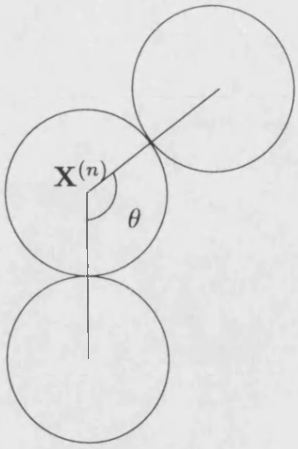

Figure 4-2: *Contact of any two discs with the nth in 2-D*

axes such that the centre of the first disc has co-ordinates (1,0). The centre of the second then has co-ordinates $(\cos\theta,\ \sin\theta)$. We have $\mathbf{J}^{(n)} = \frac{1}{2}(1+\cos\theta,\ \sin\theta)$ and so $|\mathbf{J}^{(n)}|^2 = \frac{1}{2}(1+\cos\theta)$. Thus to find the expected value of $|\mathbf{J}^{(n)}|^2$ we calculate the integral

$$\frac{\int_{\frac{\pi}{3}}^{\frac{5\pi}{3}} 1+\cos\theta d\theta}{2\int_{\frac{\pi}{3}}^{\frac{5\pi}{3}} 1 d\theta}, \tag{4.3}$$

the restricted limits ensure that there is no overlap between the two chosen and so the arrangement is physically realistic. The integral yields a value of 0.2933 and since $\alpha = 0.2933/3$, then $\alpha = 0.0978$.

Considering next an arrangement of three discs in contact with the nth, we can consider both equilibrium and non-equilibrium of the nth disc. We initially do the calculation for any arrangement of discs which may not necessarily be in equilibrium. We again let the centre of the first disc chosen have co-ordinates (1,0), that of the second have co-ordinates $(\cos\theta,\ \sin\theta)$ and that of the third have co-ordinates $(\cos\phi,\ \sin\phi)$. We require there to be no overlap between the discs and so $\frac{\pi}{3} < \theta < \frac{5\pi}{3}$, $\frac{\pi}{3} < \phi < \frac{5\pi}{3}$ and $|\theta - \phi| > \frac{\pi}{3}$. The region in which these last two discs can be chosen without overlapping either of the others is shown in figure 4-3. Solutions of no overlap are only possible in the two triangular areas containing dotted lines.

The triangle areas are symmetric and so to find the expected value of $|\mathbf{J}^{(n)}|^2$ we calculate

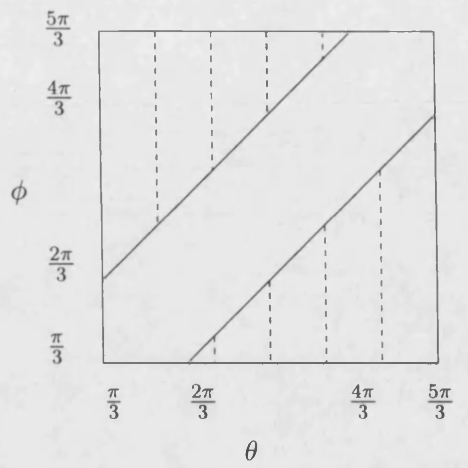

Figure 4-3: *The (θ, ϕ) region corresponding to no overlap*

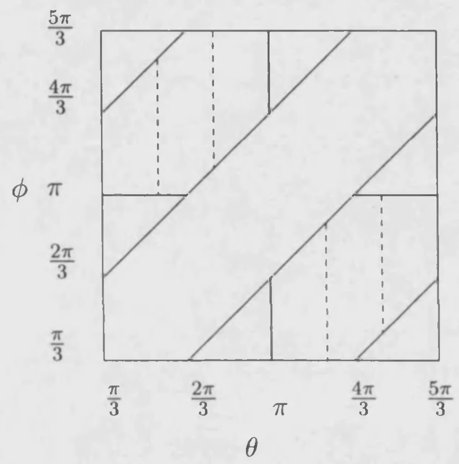

Figure 4-4: *The (θ, ϕ) region corresponding to no overlap and each disc is in equilibrium*

the integral

$$\frac{2}{9\pi^2}\int_{\theta=\frac{2\pi}{3}}^{\frac{5\pi}{3}}\int_{\phi=\frac{\pi}{3}}^{\theta-\frac{\pi}{3}}[3+2\cos\theta+2\cos\phi+2\cos(\theta-\phi)]d\theta d\phi. \tag{4.4}$$

The value of this is 0.1011 and so $\alpha = 0.1011/3 = 0.0337$.

If we now consider the random selection of three discs in contact with the nth so that the nth is in equilibrium, we find the more restricted region in which θ and ϕ can be chosen, as shown by the areas containing dotted lines in figure 4-4. The integrand is the same as above but the limits are different and we find that the expected value of $|\mathbf{J}^{(n)}|^2$ has decreased to 0.0965 and thus α=0.0965/3=0.0322.

Now we consider four discs in contact with the nth. Any chosen combination will ensure that the nth sphere is in equilibrium. We again chose our axes such that the centre of the first disc has co-ordinates (1,0), the centre of the second then has co-ordinates $(\cos\theta,\ \sin\theta)$, the third $(\cos\phi,\ \sin\phi)$ and the fourth $(\cos\psi,\ \sin\psi)$. We integrate $|\mathbf{J}^{(n)}|^2 = \frac{1}{16}[4+2(\cos\theta+\cos\phi+\cos\psi+\cos(\theta-\phi)+\cos(\theta-\psi)+\cos(\phi-\psi))]$ over the six regions:

- $\theta : \pi \to \frac{5\pi}{3},\ \phi : \frac{2\pi}{3} \to \theta - \frac{\pi}{3},\ \psi : \frac{\pi}{3} \to \phi - \frac{\pi}{3}$.
- $\theta : \pi \to \frac{5\pi}{3},\ \phi : \frac{\pi}{3} \to \theta - \frac{2\pi}{3},\ \psi : \phi + \frac{\pi}{3} \to \theta - \frac{\pi}{3}$.
- $\theta : \frac{2\pi}{3} \to \frac{4\pi}{3},\ \phi : \theta + \frac{\pi}{3} \to \frac{5\pi}{3},\ \psi : \frac{\pi}{3} \to \theta - \frac{\pi}{3}$.
- $\theta : \frac{2\pi}{3} \to \frac{4\pi}{3},\ \phi : \frac{\pi}{3} \to \theta - \frac{\pi}{3},\ \psi : \theta + \frac{\pi}{3} \to \frac{5\pi}{3}$.
- $\theta : \frac{\pi}{3} \to \pi,\ \phi : \theta + \frac{\pi}{3} \to \frac{4\pi}{3},\ \psi : \phi + \frac{\pi}{3} \to \frac{5\pi}{3}$.
- $\theta : \frac{\pi}{3} \to \pi,\ \phi : \theta + \frac{2\pi}{3} \to \frac{5\pi}{3},\ \psi : \theta + \frac{\pi}{3} \to \phi - \frac{\pi}{3}$.

This gives us an expected value for $|\mathbf{J}^{(n)}|^2$ of 0.0309 and then α=0.0103.

For six discs in contact with the nth the calculation is very simple, $\mathbf{J}^{(n)} = \mathbf{0}$ and so α=0. This is the maximum number of discs we can arrange around another in 2-D.

We have not attempted the calculation of α for five discs in contact with the nth. This is due to the fact that the integration becomes extremely cumbersome, we would need to integrate the following expression:

$$\begin{aligned}5 + 2(\cos\theta + \cos\phi + \cos\psi + \cos\xi + \cos(\theta-\phi) + \cos(\theta-\psi) + \cos(\theta-\xi)\\ + \cos(\phi-\psi) + \cos(\phi-\xi) + \cos(\psi-\xi))\end{aligned}$$

over 24 different orderings of the spheres (similar to those listed above for four discs). However, for completeness we estimate a value for α from the plot of the values of α against co-ordination number shown in figure 4-5. The '+'s on the graph represent the values of α obtained when the spheres are not in equilibrium and the 'o's the results when we do have equilibrium. We find that for five discs in contact with the nth, $\alpha \approx 0.01$.

We notice that the value of α decreases with increasing co-ordination number. This is exactly as we would expect. We have already mentioned in previous chapters that the uniform strain approximation becomes a better approximation, as the co-ordination

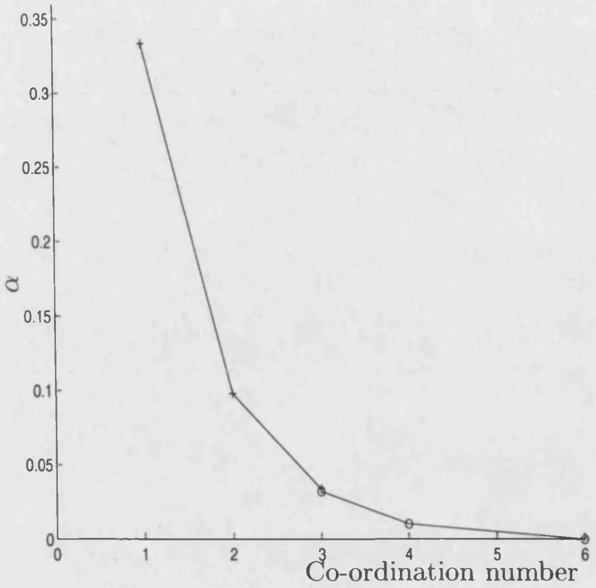

Figure 4-5: *Plot of results for α versus co-ordination number from the consideration of 2-D discs*

number increases and α represents deviation from this ideal behaviour. It therefore follows that α should decrease with increasing co-ordination number.

4.1.2 A Random Packings of Spheres

We consider the calculation of the expected values of α and χ for a random packing of equal-sized spheres. These will be the results that can be used in the theoretical work of Chapter 3 to predict modified values of the effective elastic moduli. It would be very difficult to calculate the expected value of α for spheres in three dimensional space using similar analytical methods to those above. Hence values for both α and χ must be found from a numerical average using computer simulation. Matlab was used to perform these calculations.

We use computer programs to randomly pick spheres in contact with the nth sphere. A typical example of one of these appears in Appendix B. By repeatedly running the simulation, it is possible to find an average of several hundred calculations, say, the number of calculations performed being dependent upon the time involved in each run. The more spheres to be chosen, the longer each calculation took and hence the fewer the calculations that it was possible to do within a reasonable amount of time.

Especially important in the calculations was to impose a condition of no overlap between spheres to ensure physically realistic answers. Also, for the particular results that will be used in the expressions found in Chapter 3 we require equilibrium of each sphere. However, similarly to the 2-D case, here we also consider the values obtained when the spheres are not necessarily in equilibrium. In 3-D, we require a minimum of seven spheres to ensure that any possible combination of chosen spheres are in equilibrium. However, it is possible to have several combinations of as few as four spheres in contact with the nth, such that this nth sphere is in equilibrium. We must include checks within some of our programs to find these combinations.

The general algorithm for all the programs was to pick co-ordinates (r, θ, ϕ) such that the centre of the nth sphere was at (0,0,0) and θ and ϕ defined such that the centre of the first sphere chosen in contact with this always has co-ordinates (2,0,0). Then the unit vector directed along the line of centres was (1,0,0). A second sphere was then chosen such that $\phi = 0$, but with θ picked randomly in the interval $[\pi/3, \pi]$. The remaining spheres were chosen at random, imposing the condition of no overlap which is described below.

The program asks the computer to choose a random number p say, this falls between [0,1] and so we let $\phi = 2\pi p$. Picking θ correctly requires more thought, we need to ensure that the contacting spheres are distributed with an even probability density. As we have mentioned, we want θ to be contained in the interval $[\pi/3, \pi]$ and thus $\sin\theta \in [\sqrt{3}/2, 1]$ or [1,0]. This is shown by the area to the right of the vertical line $\theta = \pi/3$ in figure 4-6. We want the values to be chosen uniformly on these intervals. The size of the area $[\theta, \theta + \delta\theta]$ is $\sin\theta\delta\theta$ and the number of values we pick in a given area must be proportional to that area. We notice that

$$\int_{\theta}^{\pi} \sin\theta d\theta = 1 + \cos\theta$$

and

$$\int_{\frac{\pi}{3}}^{\pi} \sin\theta d\theta = \frac{3}{2}.$$

From this we see that we require $1 + \cos\theta \in [0, \frac{3}{2}]$ which then gives the condition $\cos\theta \in [-1, 1/2]$. Hence, to define a random θ we let $\theta = \cos^{-1}\left\{\frac{3}{2}q - 1\right\}$, where q is a second random number within [0,1]. The unit vector $\mathbf{I}^{(nn')}$ joining the centre of the nth sphere to the n'th, is then found using $\mathbf{I}^{(nn')} = [\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta]$.

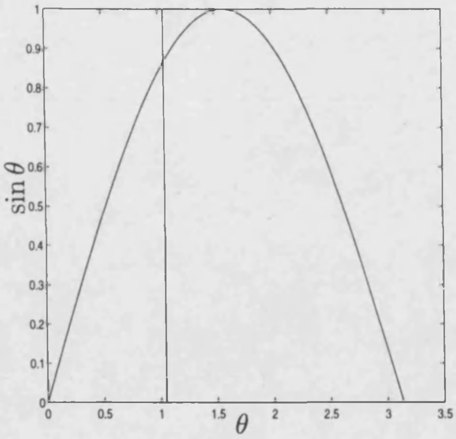

Figure 4-6: *Restricted Area Within Which to Pick* $\sin\theta$ *Uniformly*

The next part is to check that the sphere that has been chosen does not overlap with the ones already present. The way we have chosen θ for this sphere has already ensured that it does not overlap with the first sphere chosen, whose centre has co-ordinates (2,0,0). However, we must check all of the others as well. If the unit vector joining the centre of the nth sphere to a contacting one is

$$\mathbf{I1} = [\sin(\theta_1)\cos(\phi_1), \sin(\theta_1)\sin(\phi_1), \cos(\theta_1)]$$

and that of a second

$$\mathbf{I2} = [\sin(\theta_2)\cos(\phi_2), \sin(\theta_2)\sin(\phi_2), \cos(\theta_2)]$$

then we must ensure that the angle separating these two is not less than $\pi/3$. This implies that we must check the cosine of this angle is not greater than 1/2. Now, the cosine of the angle between these unit vectors is given by

$$\cos A = \sin(\theta_1)\sin(\theta_2)\cos(\phi_1 - \phi_2) + \cos(\theta_1)\cos(\theta_2)$$

and if $\cos A > 0.5$ then we throw away this last sphere. If $\cos A < 0.5$ then these particular two do not overlap, but we must also repeat the check to ensure that there is no overlap between the current sphere and any of the others either. If the current sphere overlaps with any others then we throw it away and try to choose another which does not overlap any of the others. Sometimes it can be very hard for the computer to find a 'gap' to put another sphere into. If after one hundred tries it does not succeed then we throw away all the spheres we have already chosen and start again.

This process of picking random numbers and subsequently co-ordinates for the sphere centres, is repeated until the required number of non-overlapping spheres in contact with our initial one, has been found. The vector $\mathbf{J}$ and matrix $\mathbf{N}$ are then determined, from which the the values of α and χ can be calculated. We run the program many times in order to obtain average values for α and χ.

We start with the very easy case of one sphere in contact with the nth. There is obviously no possibility of equilibrium in this situation and we have the unit vector along the line of centres of the two spheres given by (1,0,0). Thus $\mathbf{J}^{(n)} = (1,0,0)$ and hence $\alpha = 1/3$. Similarly, it is very easy to calculate $N_{ijk}^{(n)}$ the entries in which are all zero except $N_{333}^{(n)} = 1$. Thus, χ also equals 1/3.

For two spheres in contact with the nth we have no equilibrium, except for a case very similar to that for the two, 2-D discs described above. That is, if the spheres are on exactly opposite sides of the nth sphere, then the nth sphere will be in equilibrium and when we sum the two unit vectors along the lines of centres they cancel each other completely and $\mathbf{J}^{(n)} = \mathbf{0}$. We have calculated only α for this co-ordination number, its value is 0.1258. With three spheres in contact with the nth we still cannot have equilibrium in the general case and find that α takes the value 0.0602 and $\chi = 0.0794$.

For four spheres in contact with the nth, we can start to consider combinations of spheres in equilibrium as well as those not in equilibrium. Although there will be lots of cases where a randomly picked four will not be in equilibrium, these are thrown away when we wish to apply the values of α and χ to our theory. It is easy to know by looking at a picture of an arrangement of spheres whether it is in equilibrium or not. However, it is more difficult to enable the computer to make this decision.

When we have four spheres in contact with the nth, the test for equilibrium in the computer program started by selecting two of the spheres out of the four. The plane through their centres and through the centre of the nth sphere was constructed, i.e. $\mathbf{I}_{1n} \wedge \mathbf{I}_{2n}$ found (using obvious notation). The remaining two spheres are tested to see if they are on the same side of this plane by finding both $(\mathbf{I}_{1n} \wedge \mathbf{I}_{2n}).\mathbf{I}_{3n}$ and $(\mathbf{I}_{1n} \wedge \mathbf{I}_{2n}).\mathbf{I}_{4n}$ and checking if they have the same sign, in which case they are on the same side of the original plane and equilibrium would not be possible. This was repeated for every possible combination of selection of the first pair. If the signs of the two dot products involving the remaining spheres are different for any of these combinations, then the four randomly selected spheres are not one-sided and equilibrium is possible.

For four spheres we have to find $sgn(\mathbf{I}_{1n} \wedge \mathbf{I}_{2n}.\mathbf{I}_{3n}) = s_1$, $sgn(\mathbf{I}_{1n} \wedge \mathbf{I}_{2n}.\mathbf{I}_{4n}) = s_2$, $sgn(\mathbf{I}_{1n} \wedge \mathbf{I}_{3n}.\mathbf{I}_{4n}) = s_3$ and $sgn(\mathbf{I}_{2n} \wedge \mathbf{I}_{3n}.\mathbf{I}_{4n}) = s_4$. The condition for the four spheres not one-sided is that the sequence s_1, s_2, s_3 and s_4 alternates in sign. If it did not alternate the four spheres were discarded and the whole process repeated until a selection was found that were not one-sided. The values of $J_i^{(n)}$ and $N_{ijk}^{(n)}$ were then calculated. The value of α for spheres in equilibrium was 0.0158. That of χ was 0.0457. Considering also the selection of any four spheres which may not be in equilibrium $\alpha = 0.0311$.

We next consider the selection of five spheres which ensure the initial one with which they are in contact is in equilibrium. There will be fewer cases of no equilibrium than when we only choose four spheres. To test for equilibrium with five spheres, the above algorithm can again be used by selecting four of the five and testing these for one-sidedness. If all combinations of four that can be chosen are one-sided, then all five are one-sided. If any four are not one-sided, then all five are not one-sided. These result in ten conditions on the signs of the dot products calculated, but these can be reduced. Setting up a 5X5 table with the diagonal elements blank, (see below), where $s_{12} = sgn(\mathbf{I}_{3n} \wedge \mathbf{I}_{4n}.\mathbf{I}_{5n})$, $s_{13} = sgn(\mathbf{I}_{2n} \wedge \mathbf{I}_{4n}.\mathbf{I}_{5n})$ etc., the conditions reduce to finding an alternating row in the table.

	s_{12}	s_{13}	s_{14}	s_{15}
s_{12}		s_{23}	s_{24}	s_{25}
s_{13}	s_{23}		s_{34}	s_{35}
s_{14}	s_{24}	s_{34}		s_{45}
s_{15}	s_{25}	s_{35}	s_{45}	

Running the program with these equilibrium conditions and discarding any combinations which do not satisfy the criterion above we find $\alpha = 0.0132$. We have only calculated χ when each sphere is in equilibrium and we find that $\chi = 0.0300$. If we do not restrict our choice of spheres purely to those in equilibrium we obtain $\alpha = 0.0173$.

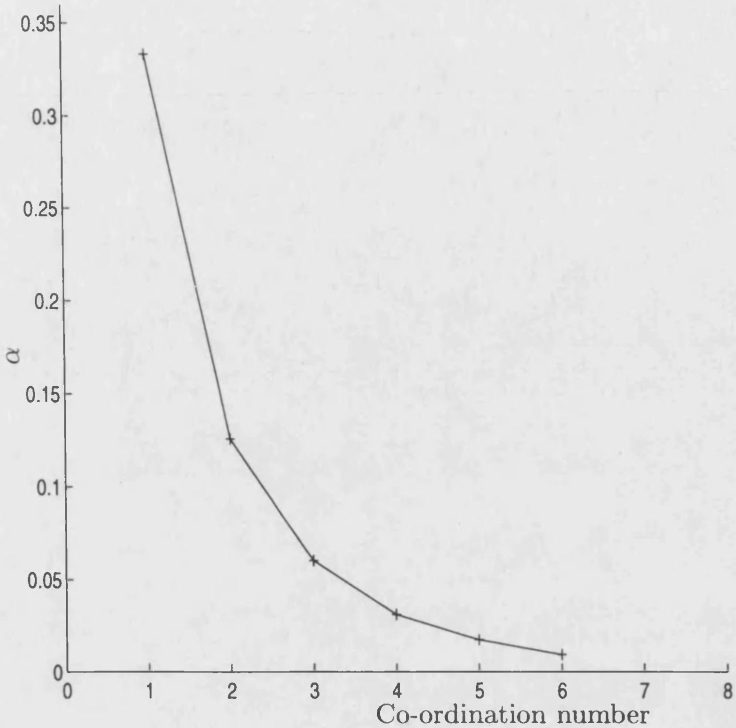

Figure 4-7: *Plot of results for α versus co-ordination number from the consideration of 3-D spheres*

For six spheres, there are fifteen conditions to ensure equilibrium if we chose two spheres out of the six and draw the plane through their centres, checking the remaining four to see if they are one-sided (this is the extension of what was described previously for four spheres). Fifteen checks would also have to be done if we chose combinations of four spheres again, extending the method used for five. Since there are now few combinations that will be one-sided the quickest way of checking is to use the former fifteen conditions, each will not have to be checked every time the program is run, as soon as one is found to be untrue then we know that the spheres are not one-sided. In the case of picking combinations of four, every condition would have to be checked each time. Now, α takes a value of 0.0093 when there are no equilibrium restrictions and 0.0091 with. The first of these values is plotted along with the other values of α when there are no equilibrium conditions imposed, against co-ordination number in figure 4-7. These values obtained from six spheres confirm the fact that few combinations are still one-sided since these values are not significantly different. Again, we only calculate χ with equilibrium conditions imposed, the simulation yields a value of 0.0190. A graph of the values of χ against co-ordination number are shown in figure 4-8, the spheres

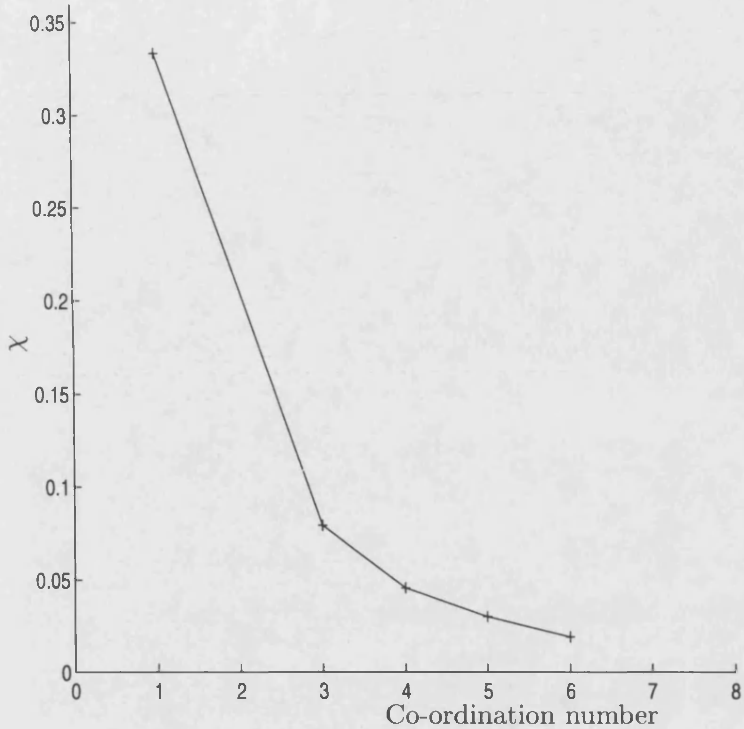

Figure 4-8: *Plot of results for χ versus co-ordination number from the consideration of 3-D spheres*

will be in equilibrium except in the case of a co-ordination number between one and three, inclusive.

Once the number of spheres selected gets to seven or more, all of the combinations chosen will be in equilibrium. For seven and eight spheres the value of α was therefore calculated without checking for equilibrium, α was found to have a value of 0.0055 for seven spheres and 0.0042 for eight.

For nine, ten and eleven spheres in contact with the nth the computer programs take progressively more time to calculate a single value for α, this can as long as several hours. Hence it is not practical to try and run the program many hundreds of times to obtain an average. However, in the case of twelve spheres we have the simple result that α=0. Hence we could estimate the missing values for these other three cases if we so wished from the graph of results for α shown in figure 4-9. This graph shows the values obtained when our initial sphere is in equilibrium. It can be seen that the curve does not pass perfectly through the plotted points but this is probably because the values have not been calculated with the same accuracy. We mentioned previously

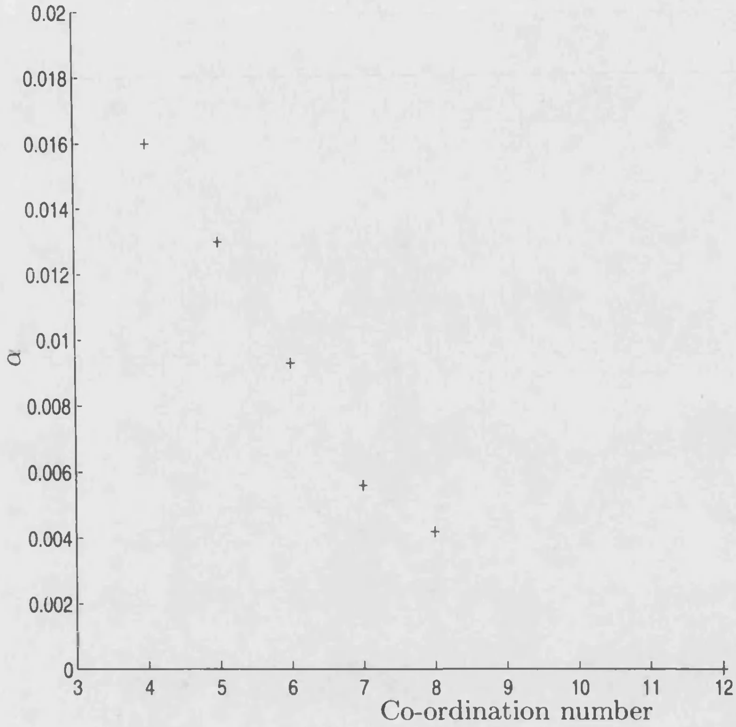

Figure 4-9: *Plot of results for α versus co-ordination number from the consideration of 3-D spheres in equilibrium*

the fact that as the number of spheres that the computer must choose increases, the programs become slower and slower to run. Thus for a co-ordination number of eight it was only practical to run the simulation a few tens of times, whereas for a co-ordination number of four it was practical to run the program for thousands of arrangements.

All these values are approximate since, as we mention above, some of the calculations took so long to complete that it was not possible to repeat them as many times as some of the others. However, the general pattern seen in the values of α that we had for 2-D discs, can be seen again here, that is decreasing α with increasing number of contacts. This is true for both the values where equilibrium conditions were ignored and those where they were included. We also note that χ decreases with increasing co-ordination number.

4.1.3 Fixing Three Spheres in Contact with the nth

For interest, we also ran some further simulations to find numerical values for α when the spheres in contact with the nth were not all randomly chosen by the computer. We

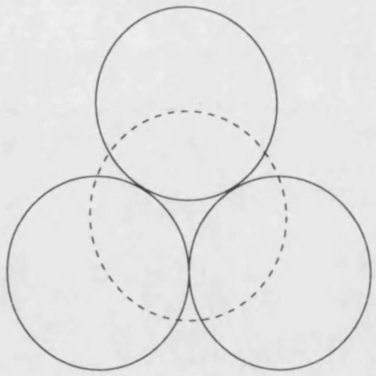

Figure 4-10: *Fix the Positions of Three Spheres in Contact with the* nth

wished to see what effect this would have upon the numerical values of the parameters and hence how the predicted values of the effective elastic moduli were effected. We considered a particular example of a possible arrangement of spheres in contact with the nth. We take the first three spheres in contact with the nth, also in contact with each other. This gives us an arrangement like that in figure 4-10, where we are looking from below these three spheres. The dotted circle represents the outline of the nth sphere which lies above the three spheres shown by the circles with solid outline. Thus, we pick our axes such that if the centre of the nth sphere is at (0,0,0) then we fix the position vectors of the centres of these other three spheres at $(\frac{2\sqrt{(3)}}{3}, 0, \frac{2\sqrt{(6)}}{3})$, $(-\frac{\sqrt{(3)}}{3}, 1, \frac{2\sqrt{(6)}}{3})$ and $(-\frac{\sqrt{(3)}}{3}, -1, \frac{2\sqrt{(6)}}{3})$ in cartesian co-ordinates.

The required number of remaining spheres in contact with the nth are then chosen randomly as before, ensuring no overlap with any of the others and checking to ensure equilibrium when appropriate. This arrangement of contacting spheres is highly unlikely to occur in the simulations, although it seems quite reasonable to think that it might occur in real packings. We do not have any idea as to what percentage of spheres within a packing might be arranged like this, but we shall speculate about some possible values near the end of this chapter and calculate the new theoretical predictions for the moduli.

For five spheres in contact with the nth sphere, the new value of α is 0.0344 as compared with 0.0132 for five chosen randomly. For six we have 0.0328 as compared with 0.0091 and for seven, $\alpha = 0.0127$, compared with 0.0055 from earlier. Thus α is significantly larger for this arrangement with three fixed spheres in contact with the nth, compared with that of a randomly chosen group.

4.2 Comparison Between Theory and Numerical Simulations

We re-write our new expressions for all the moduli found in Chapter 3, equations (3.67) and (3.68), using the notation of Jenkins *et al.* [43]. This is for easy comparison between our new expressions and the Lamé moduli found in equations (32) and (33) and also the bulk modulus of Jenkins' paper. Jenkins' equations (32) and (33) are actually the same as the expressions found previously by Walton [86] but re-written for the purposes of Jenkins' work. For a packing of infinitely rough spheres we have the following expressions for the effective shear modulus and effective bulk modulus, respectively,

$$\mu^* = \frac{2}{5\pi}\frac{\mu k v}{(1-\nu)}\left[\frac{3}{16}\frac{(1-\nu)P}{\sigma^2\mu}\right]^{1/3}\frac{(5-4\nu)}{(2-\nu)} \tag{4.5}$$

and

$$\kappa^* = \frac{2}{3\pi}\frac{\mu k v}{(1-\nu)}\left[\frac{3}{16}\frac{(1-\nu)P}{\sigma^2\mu}\right]^{1/3}. \tag{4.6}$$

These equations include Poisson's ratio, ν, co-ordination number, k, solid fraction, v, average contact force P, sphere diameter, σ and the shear modulus of the material μ. We represent our new theoretical expressions in terms of these parameters:

$$\begin{aligned}\mu^* \;=\;& \frac{2}{5\pi}\frac{\mu k v}{(1-\nu)}\left[\frac{3}{16}\frac{(1-\nu)P}{\sigma^2\mu}\right]^{1/3}\frac{(5-4\nu)}{(2-\nu)}\\ &\left\{1-\frac{1}{(14+3\nu-11\nu^2)}\Big(9(2+\nu-\nu^2)(30+7\nu-23\nu^2)\right.\\ &\qquad +\frac{72}{5}(12+2\nu-10\nu^2)(5+\nu-4\nu^2)\Big)\,\alpha\\ &\qquad\left.-\frac{54\nu^2(1+\nu)^2}{10(6+\nu-5\nu^2)(5+\nu-4\nu^2)}(10\chi-3\alpha)\right\}\end{aligned} \tag{4.7}$$

and

$$\kappa^* \;=\; \frac{2}{3\pi}\frac{\mu k v}{(1-\nu)}\left[\frac{3}{16}\frac{(1-\nu)P}{\sigma^2\mu}\right]^{1/3}\left\{1-\frac{27(2+\nu-\nu^2)(26+5\nu-21\nu^2)}{(14+3\nu-11\nu^2)^2}\right\}\alpha. \tag{4.8}$$

Taking Poisson's ratio $\nu = 0.21$, coordination number $k = 5.36$, solid fraction, $v = 0.63$, average contact force $P = 7\text{x}10^{-3}$N and average sphere diameter, $\sigma = 0.22$mm, from Walton's theory using equation (4.6), the bulk modulus is calculated to be 245MPa.

The shear modulus from equation (4.5) is 338MPa. However, Jenkins *et al.* [43] found values of 185MPa and 127MPa respectively for these moduli from the numerical simulations. We cannot specifically calculate α or χ and hence recalculate the theoretical predictions using our new expressions, for a coordination number of 5.36. Instead, we use the values found for coordination numbers 5 and 6 and estimate a value of α from the graph in figure 4-9. Alternatively, this could be calculated from the values given by 4, 5, 6 and 7 contacts and then weighted so as to give $\eta = 5.36$. As we have not calculated a value for χ when there are 7 contacts, we estimate its value when $\eta = 5.36$, by assuming that its value linearly decreases as the co-ordination number increases from 5 to 6. Then we can say $\alpha \approx 0.012$ and $\chi \approx 0.026$. Now from equations (4.8) and (4.7), we calculate that $\kappa^* = 223$MPa, which is a reduction of 9% on the previous theoretical value and $\mu^* = 308$MPa, a reduction of 9%.

The results are summed up in the following table.

Modulus	Jenkins Simulations	Walton's Theory	New Theory
Bulk	185MPa	245MPa	223MPa
Shear	127MPa	338MPa	308MPa

These new theoretical results are slightly closer to those of the numerical simulation, although the theoretical shear modulus is still more than twice that of the simulation. Obviously just modifying the uniform strain approximation to first order is not good enough to resolve the difference between these results which are so inconsistent. Further reasons are investigated and disussed in the following two chapters.

These are all results for infinitely rough spheres, the same methods can be used to calculate the moduli for perfectly smooth spheres. In this second case the expression for the bulk modulus was found, by Walton [86], to be the same as that when the spheres were rough. Our new results however predict that the expression for the bulk modulus in this case is

$$\kappa^* = \frac{2}{3\pi}\frac{\mu k v}{(1-\nu)}\left[\frac{3}{16}\frac{(1-\nu)P}{\sigma^2\mu}\right]^{1/3}\{1-15\alpha\}. \tag{4.9}$$

Again, taking $\alpha = 0.012$ and other values as given in Jenkins *et al.* [43] we see a 18% reduction of the bulk modulus found by Walton [86], which gives $\kappa^* = 201$MPa. It is interesting to note that this value is much closer to that found by Jenkins *et al.* [43], than the one found by considering the infinitely rough spheres. However, we cannot expect to model these simulations by smooth spheres when the coefficient of friction used was 0.3.

As we have already mentioned, α increases with decreasing co-ordination number. Hence, the effective elastic moduli will decrease as the average number of contacts decreases. This is consistent with what we have said about the uniform strain approximation - it becomes less accurate as the contact number decreases. Hence we would expect our correction term to produce larger changes in the effective moduli for low co-ordination values.

Variation on the Arrangement of Spheres

We return to consider the case of our three fixed spheres as discussed in section 4.1.3. If the spheres were all arranged in the packing as described in that section, then for a packing where the average contact number is 5.36, as in the one in Jenkins work and discussed in the previous section, we find that the new value for α would be 0.0337. This is again derived by considering the values found for 5 and 6 contacts and assuming that the value of alpha decreases linearly between these two.

Now, if we guess that there might be 5% of the spheres in the packing with this feature then combining this with our previous value for α we obtain the new value, $\alpha = 0.013$. If we recalculate the effective bulk modulus using this value of α there will clearly be a decrease in the values that we have already calculated. We have not investigated what effect this packing arrangement would have on the value of χ so we just consider the bulk modulus. We find a modified value of κ^* =220MPa. There is obviously no vast difference between this and the value calculated in the previous section. However, if we increase our guess to 10% of spheres in the packing with this property, then we now find $\alpha = 0.014$ and κ^* =218MPa and we have reduced the bulk modulus by around 11% as compared with the 9% of the previous section. It may be properties of the packing, such as this, that yield lower effective moduli than we have been able to calculate thus far. This particular arrangement seems to have little effect upon the values of the moduli and we do not have any data with respect to the proportion of contacts that may be like this. Unfortunately we cannot, therefore, draw any firm conclusions.

4.2.1 Discussion and Conclusions

We have improved the correlation between the values for the bulk and shear moduli as predicted by Walton's work with the uniform strain approximation and those predicted by the numerical simulations discussed in Jenkins *et al* [43].

We have used a perturbation of the uniform strain approximation as a first step. The shear modulus was initially almost 3 times that found by numerical simulation and so a small reduction in this of about 9%, will still not enable the theory to predict its value accurately. However, as the reduction required to improve the predicted bulk modulus was around 25% we have made a significant change with our perturbation. We reduced the value predicted for infinitely rough spheres by around 9% and that for perfectly smooth spheres by 18%. Unfortunately, although the prediction is closest to the numerical results using the smooth sphere calculations, it would be difficult to justify modelling the experimental glass spheres, as smooth spheres, since their coefficient of friction was 0.3.

Indeed, in order to find a value of 185MPa for the bulk modulus, κ^*, from our new theoretical expressions we would need a value of $\alpha \approx 0.033$, which is more than twice the value we have calculated in this chapter. Using the theoretical expression for the shear modulus and substituting for this value of α, we find a 25% reduction such that $\mu^* = 256$MPa. So, with this value of α, even though we have the exact value for the bulk modulus, the shear modulus is still double that calculated in the simulations.

We believe there are some reasons why we would not expect the theoretical results to be identical to the experiments and simulations. In the work by Jenkins *et al.* [43] the spheres considered are not all of equal size, with one sphere of average diameter 0.37mm for every ten of average diameter 0.22mm. Although this is a relatively small number of large spheres and is purely to prevent regular arrangements of the smaller spheres, we believe this could effect the results. The work in the next two chapters investigates the possible implications of the different sizes.

A second reason is connected to the coordination number. We would expect the uniform strain approximation to be accurate where there is a large coordination number. Equation (3.5) becomes less accurate as the coordination number decreases, to be consistent with Jenkins *et al.* [43] we have taken between 5 and 6 contacts to be the average. This might suggest that our perturbations of the approximation are not so small as we have assumed and maybe second order terms should also be considered.

Some further work has been done recently by Jenkins, in collaboration with Koenders, this was presented at the Powders and Grains '97 conference, Jenkins and Koenders [44]. They, like us, have tried to find a different way to tackle this problem and to determine why the theory and numerical simulations predict inconsistent results. Their paper does not actually give any completed calculations, but discusses an alternative method to the uniform strain approximation, for obtaining the incremental stress-strain relationship required to determine the effective elastic moduli for a heterogeneous medium. They study small local assemblies of identical discs and consider a pair in contact. To find a solution for the increments in the translations of the centres of the two discs and the rotations about their centres, they too consider force and moment equilibrium when all the surrounding discs are constrained to move in accordance with the uniform strain approximation. Unfortunately this is just a suggested method, these calculations have not been completed as yet, so we do not know whether the theoretical predictions are closer to those of the numerical simulation or not.

Koenders [48] has also questioned the use of mean field theories such as the uniform strain approximation, although not within the context that we are working. His paper is based upon methods described in Koenders [47] and concludes that such approximations are acceptable at low stress ratios when the sphere contacts 'stick'. However, he claims that for high stress ratios, (which he measures by the onset of slip), heterogenous effects must be included.

Both of these pieces of work still concentrate upon packings of equal sized spheres. In the chapters that follow we extend our work to cover dense, random, binary packings of spheres.

Chapter 5

A Random Binary Packing of Spheres

As mentioned in chapter 3, we believe it is possible that a few large spheres in a packing of small spheres, could affect the values of the moduli. In both their experiments and numerical simulations Jenkins *et al.* [43] use random binary packings, a few larger spheres are included to prevent regular packings of the small. We also now include this size difference into the existing theory and use some numerical calculations by Dr. Luc Oger [62], to see how this affects the values of the effective elastic moduli. We hope to discover a closer correlation between theoretical predictions and numerical results.

In order to find a first approximation, we begin in this chapter by assuming that when the initial compression is applied to the packing, the spheres are still displaced in accordance with the uniform strain approximation. We derive expressions for the effective bulk and shear moduli, using the same methods as before. Once we have found these, we proceed in the next chapter to consider a perturbation of this approximation, in the same way that we have already done with a packing of equal sized spheres in Chapter 3.

5.1 Oblique Contact of Different Sized Spheres in Contact

In his book, Johnson [46] considers the geometry of non-conforming bodies in contact, this is discussed in section 1.2.6. We use these results to calculate the geometry of two spheres of different radii in contact.

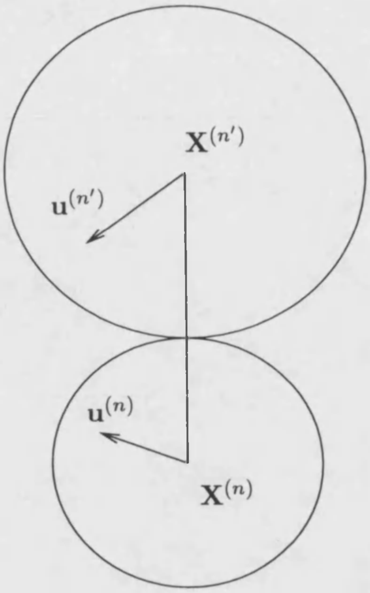

Figure 5-1: *Initial Deformation of Two Spheres of Different Size in Contact*

First, we define R' in terms of the two radii, R_l, the radius of the large sphere and R_s, that of the small sphere by

$$\frac{1}{R'} = \frac{1}{R_l} + \frac{1}{R_s}, \tag{5.1}$$

so that

$$R' = \frac{R_l R_s}{R_l + R_s}. \tag{5.2}$$

Some contacts in the packing will be between spheres of the same size and in this case all of the previous theory still holds. However, there will also be contacts between spheres of different size and in the work that follows, we extend the theory to cover this situation.

Consider the oblique compression of two spheres in contact initially at a point, one sphere is large, the other small (see figure 5-1). We let the initial contact point be the origin of our rectangular cartesian axes and such that the z-axis is directed along the line of centres into the lower sphere. The spheres are compressed together such that the centre of the larger sphere has undergone a displacement $(u_{(l)0}, v_{(l)0}, w_{(l)0})$ and the centre of the smaller a displacement $(-u_{(s)0}, -v_{(s)0}, -w_{(s)0})$. Since we have imposed a compression on the spheres a contact area will form, the size of which is small in comparison with the size of the bodies.

Using the results of Section 1.2.6, we recall that the points within the contact area of each sphere must satisfy:

$$w_{(s)} + w_{(l)} = \delta - Ax^2 - By^2 \tag{5.3}$$

where δ is the initial separation of the two surfaces, $w_{(s)}$ and $w_{(l)}$ are the displacements of the surfaces points within the contact area on the bodies. The constants A and B can be determined from the following relationships, equations (1.25):

$$\begin{aligned}
A+B &= \frac{1}{2}\left(\frac{1}{R''}+\frac{1}{R'''}\right) = \frac{1}{2}\left(\frac{1}{R_1''}+\frac{1}{R_1'''}+\frac{1}{R_2''}+\frac{1}{R_2'''}\right) \\
|A-B| &= \frac{1}{2}\left\{\left(\frac{1}{R_1''}-\frac{1}{R_1'''}\right)^2+\left(\frac{1}{R_2''}-\frac{1}{R_2'''}\right)^2\right. \\
&\qquad \left. +2\left(\frac{1}{R_1''}-\frac{1}{R_1'''}\right)\left(\frac{1}{R_2''}-\frac{1}{R_2'''}\right)\cos 2\theta\right\}^{1/2}.
\end{aligned} \tag{5.4}$$

where R'' and R''' are the principal relative radii of curvature. Hence for two spheres in contact and of different size, we find

$$A = B = \frac{1}{2}\left(\frac{1}{R_s}+\frac{1}{R_l}\right). \tag{5.5}$$

Using the same techniques as in Chapter 1 we can then find, similarly to equation (1.45), that the radius of the contact area is given by

$$a^2 = R'(w_{(l)0} + w_{(s)0}). \tag{5.6}$$

In the case of infinitely rough spheres, the distribution of traction (P, Q, N) acting on the smaller (lower) sphere over the contact area has the form:

$$\begin{aligned}
P_0 &= -\frac{2(u_{(l)0}+u_{(s)0})}{\pi^2 R'(2B+C)(w_{(l)0}+w_{(s)0})}(a^2-r^2)^{1/2}, \\
Q_0 &= -\frac{2(v_{(l)0}+v_{(s)0})}{\pi^2 R'(2B+C)(w_{(l)0}+w_{(s)0})}(a^2-r^2)^{1/2}, \\
N_0 &= \frac{1}{\pi^2 R' B}(a^2-r^2)^{1/2}
\end{aligned} \tag{5.7}$$

where $r = \sqrt{(x^2+y^2)}$. The constants B and C are as defined previously, that is

$$B = \frac{1}{4\pi}\left\{\frac{1}{\mu}+\frac{1}{\lambda+\mu}\right\}$$

$$C = \frac{1}{4\pi}\left\{\frac{1}{\mu} - \frac{1}{\lambda+\mu}\right\}$$

and λ and μ are the Lamé moduli for the material. These are the analogous results to equation (1.47). The tractions acting on the upper (large) sphere due to its contact with the lower (small) sphere are equal and opposite to these.

We actually require the total force acting across the contact area and this is found by integrating the expressions in equation (5.7) and is denoted by $(\overline{P}, \overline{Q}, \overline{N})$. We find that

$$\begin{aligned}\overline{P} &= \frac{4(u_{(l)0} + u_{(s)0})(R'(w_{(l)0} + w_{(s)0}))^{1/2}}{3\pi(2B+C)}, \\ \overline{Q} &= \frac{4(v_{(l)0} + v_{(s)0})(R'(w_{(l)0} + w_{(s)0}))^{1/2}}{3\pi(2B+C)}, && (5.8) \\ \overline{N} &= \frac{2R'^{1/2}(w_{(l)0} + w_{(s)0})^{3/2}}{3\pi B}. && (5.9)\end{aligned}$$

As has been discussed several times already in this thesis, in the calculation of the effective elastic moduli we need expressions for the incremental forces acting. Thus, we now consider a further incremental displacement of the centre of the larger sphere, $(\delta u_{(l)0}, \delta v_{(l)0}, \delta w_{(l)0})$ and again the smaller one has a displacement in the opposite direction with components $(-\delta u_{(s)0}, -\delta v_{(s)0}, -\delta w_{(s)0})$. The contact area is still circular and now has radius b, where

$$b^2 = R'(w_{(l)0} + w_{(s)0} + \delta w_{(l)0} + \delta w_{(s)0}). \qquad (5.10)$$

The problems for the two separate cases $\delta w_0 > 0$ (compression) and $\delta w_0 < 0$ (unloading) are solved and if $\delta w_0 < 0$, then it is so small that contact is not lost. The new force distribution will have the form $(P+\delta P, Q+\delta Q, N+\delta N)$. The normal component, which is the same whatever the sign of δw_0 is given by:

$$N_0 + \delta N = \frac{2}{\pi^2 R' B}(b^2 - r^2)^{1/2} \qquad (5.11)$$

where b is the radius of the new circular contact area, as given above.

Considering first the case of $\delta w_0 < 0$, the tangential tractions are calculated to be

$$\begin{aligned}
P_0 + \delta P &= \frac{1}{\pi^2 R'(2B+C)(w_{(l)0}+w_{(s)0})}\{2(u_{(l)0}+u_{(s)0})(b^2-r^2)^{1/2} \\
&\quad +(a^2(u_{(l)1}+u_{(s)1}) - b^2(u_{(l)0}+u_{(s)0}))(b^2-r^2)^{-1/2}\}, \\
Q_0 + \delta Q &= \frac{1}{\pi^2 R'(2B+C)(w_{(l)0}+w_{(s)0})}\{2(v_{(l)0}+v_{(s)0})(b^2-r^2)^{1/2} \\
&\quad +(a^2(v_{(l)1}+v_{(s)1}) - b^2(v_{(l)0}+v_{(s)0})(b^2-r^2)^{-1/2}\} \qquad (5.12)
\end{aligned}$$

where $u_{(l)1} = u_{(l)0} + \delta u_{(l)0}$, $u_{(s)1} = u_{(s)0} + \delta u_{(s)0}$, $v_{(l)1} = v_{(l)0} + \delta v_{(l)0}$ and $v_{(s)1} = v_{(s)0} + \delta v_{(s)0}$. Hence, by integrating these equations an expression for the total force acting across the contact area may be obtained, from which we find that the total incremental forces acting are:

$$\begin{aligned}
\overline{\delta P} &= \frac{2}{3\pi R'(2B+C)(w_{(l)0}+w_{(s)0})}\left\{3a^2 b(\delta u_{(l)0}+\delta u_{(s)0})\right. \\
&\qquad \left. -(a-b)^2(2a+b)(u_{(l)0}+u_{(s)0})\right\}, \\
\overline{\delta Q} &= \frac{2}{3\pi R'(2B+C)(w_{(l)0}+w_{(s)0})}\left\{3a^2 b(\delta v_{(l)0}+\delta v_{(s)0})\right. \\
&\qquad \left. -(a-b)^2(2a+b)(v_{(l)0}+v_{(s)0})\right\}, \\
\overline{\delta N} &= \frac{2(b^3-a^3)}{3\pi R'B}. \qquad (5.13)
\end{aligned}$$

For the second case, if $\delta w_0 > 0$, then the contact area increases in size and we find that

$$\begin{aligned}
P_0 + \delta P &= \frac{2}{\pi^2 R'^2(2B+C)(w_{(l)0}+w_{(s)0})(\delta w_{(l)0}+\delta w_{(s)0})}\{b^2(u_{(l)0}+u_{(s)0}) \\
&\quad -a^2(u_{(l)1}+u_{(s)1}))(a^2-r^2)^{1/2} + (u_{(l)1}+u_{(s)1}-u_{(l)0}-u_{(s)0})a^2(b^2-r^2)^{1/2}\}, \\
Q_0 + \delta Q &= \frac{2}{\pi^2 R'^2(2B+C)(w_{(l)0}+w_{(s)0})(\delta w_{(l)0}+\delta w_{(s)0})}\{b^2(v_{(l)0}+v_{(s)0}) \\
&\quad -a^2(v_{(l)1}+v_{(s)1}))(a^2-r^2)^{1/2} + (v_{(l)1}+v_{(s)1}-v_{(l)0}-v_{(s)0})a^2(b^2-r^2)^{1/2}\}, \\
N_0 + \delta N &= \frac{1}{\pi^2 R'B}(b^2-r^2)^{1/2}. \qquad (5.14)
\end{aligned}$$

Then the total incremental forces acting are given by,

$$\begin{aligned}
\overline{\delta P} &= \frac{4(b^3-a^3)(\delta u_{(l)0}+\delta u_{(s)0})}{3\pi R'(2B+C)(\delta w_{(l)0}+\delta w_{(s)0})}, \\
\overline{\delta Q} &= \frac{4(b^3-a^3)(\delta v_{(l)0}+\delta v_{(s)0})}{3\pi R'(2B+C)(\delta w_{(l)0}+\delta w_{(s)0})},
\end{aligned}$$

$$\overline{\delta N} = \frac{2(b^3 - a^3)}{3\pi R' B}. \tag{5.15}$$

In general, the expressions for both $\overline{\delta P}$ and $\overline{\delta Q}$ will differ. However, in the case of the increment being infinitesimal, these both reduce to the same form and we have

$$\overline{\delta P} = \frac{2(R'(w_{(l)0} + w_{(s)0}))^{1/2}(\delta u_{(l)0} + \delta u_{(s)0})}{\pi(2B + C)},$$
$$\overline{\delta Q} = \frac{4(R(w_{(l)0} + w_{(s)0}))^{1/2}(\delta v_{(l)0} + \delta v_{(s)0})}{\pi(2B + C)} \tag{5.16}$$

and also

$$\overline{\delta N} = \frac{2(R'(w_{(l)0} + w_{(s)0}))^{1/2}(\delta w_{(l)0} + \delta w_{(s)0})}{\pi B}. \tag{5.17}$$

These are the results for infinitely rough spheres.

In the case of perfectly smooth spheres there will be no shear traction across the contact area. Thus the total force acting at the end of the initial deformation will be

$$\overline{P} = \overline{Q} = 0, \tag{5.18}$$

and

$$\overline{N} = \frac{2(R')^{1/2}(w_{(l)0} + w_{(s)0})^{3/2}}{3\pi B} \tag{5.19}$$

and the incremental forces will be

$$\overline{\delta P} = \overline{\delta Q} = 0, \tag{5.20}$$

and

$$\overline{\delta N} = \frac{(R'(w_{(l)0} + w_{(s)0}))^{1/2}(\delta w_{(l)0} + \delta w_{(s)0})}{\pi B}. \tag{5.21}$$

5.2 Initial Compressive Force Applied to the Boundary

As we have done several times, we now continue by considering the packing as a whole. The initial deformed configuration is attained by the application of a displacement on the boundary of the packing, $\mathbf{u}$. This is consistent with a uniform compressive strain, i.e. $u_i = e_{ij}x_j$, and leads to a displacement of the centre of the nth sphere whose centre has position vector $\mathbf{X}^{(n)}$.

Let the displacement of this nth sphere be $\mathbf{u}^{(n)}$ and consider a second sphere, n', in contact with the nth. In the case that both of these spheres are of equal size, either both small or both large, then the position vector of their contact point is $\frac{1}{2}(\mathbf{X}^{(n)}+\mathbf{X}^{(n')})$ and this undergoes a displacement $\frac{1}{2}(\mathbf{u}^{(n)}+\mathbf{u}^{(n')})$. Relative to this point, the displacements of the sphere centres are $\frac{1}{2}(\mathbf{u}^{(n)}-\mathbf{u}^{(n')})$ and $\frac{1}{2}(\mathbf{u}^{(n')}-\mathbf{u}^{(n)})$ for the nth and n'th spheres respectively. These are as previously discussed in Chapter 1. However, if the spheres are different sizes, then with the nth sphere small say and the n'th large we find that the position vector of the contact point is now given by

$$\frac{1}{(R_l+R_s)}\left(R_l\mathbf{X}^{(n)}+R_s\mathbf{X}^{(n')}\right) \tag{5.22}$$

and upon application of the deformation on the boundary, the displacement it undergoes is

$$\frac{1}{2}(\mathbf{u}_{(s)}^{(n)}+\mathbf{u}_{(l)}^{(n')}). \tag{5.23}$$

Relative to this point, the displacement of the centre of the small sphere, n, is

$$\frac{1}{2}(\mathbf{u}_{(s)}^{(n)}-\mathbf{u}_{(l)}^{(n')}) \tag{5.24}$$

and that of the large sphere, n', is

$$\frac{1}{2}(\mathbf{u}_{(l)}^{(n')}-\mathbf{u}_{(s)}^{(n)}). \tag{5.25}$$

We continue by using the subscripts (l) and (s) to represent quantities relating to large and small spheres respectively. The extra brackets are inserted to try to avoid confusion with component indices, although these will not be included for scalar quantities such as R_s. Hence, the displacement of the centre of the nth sphere is $\mathbf{u}_{(s)}^{(n)}$ for a small sphere and $\mathbf{u}_{(l)}^{(n)}$ for a large sphere. To find the expression for the total force acting on the nth sphere due to its contact with another, we must also redefine the unit vector directed along their line of centres. For two small spheres in contact this is given by:

$$l_{(ss)i}^{(nn')}=\frac{X_{(s)i}^{(n)}-X_{(s)i}^{(n')}}{2R_s} \tag{5.26}$$

and similarly, for two large spheres in contact it is given by

$$I_{(ll)i}^{(nn')} = \frac{X_{(l)i}^{(n)} - X_{(l)i}^{(n')}}{2R_l}. \tag{5.27}$$

We will also have the contacts between large and small spheres and the unit vector directed along the line of centres in this case will be

$$I_{(sl)i}^{(nn')} = \frac{X_{(s)i}^{(n)} - X_{(l)i}^{(n')}}{R_l + R_s}. \tag{5.28}$$

Now using the results of Chapter 1, the total force acting on the nth small sphere due to its contact with another small sphere n' is given by:

$$\begin{aligned} \mathbf{F}_{(ss)}^{(nn')} &= \frac{(2R_s)^{1/2}}{3\pi B(2B+C)}\{2B[(\mathbf{u}_{(s)}^{(n')} - \mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(ss)}^{(nn')}]^{1/2}(\mathbf{u}_{(s)}^{(n')} - \mathbf{u}_{(s)}^{(n)} \\ &\quad +(\omega_{(s)}^{(n')} + \omega_{(s)}^{(n)}) \wedge R_s\mathbf{I}_{(ss)}^{(nn')}) + C[(\mathbf{u}_{(s)}^{(n')} - \mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(ss)}^{(nn')}]^{3/2}\mathbf{I}_{(ss)}^{(nn')}\} \end{aligned} \tag{5.29}$$

and the total force acting on the nth large sphere, due to its contact with the n'th large is

$$\begin{aligned} \mathbf{F}_{(ll)}^{(nn')} &= \frac{(2R_l)^{1/2}}{3\pi B(2B+C)}\{2B[(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(l)}^{(n)}).\mathbf{I}_{(ll)}^{(nn')}]^{1/2}(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(l)}^{(n)} \\ &\quad +(\omega_{(l)}^{(n')} + \omega_{(l)}^{(n)}) \wedge R_l\mathbf{I}_{(ll)}^{(nn')}) + C[(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(l)}^{(n)}).\mathbf{I}_{(ll)}^{(nn')}]^{3/2}\mathbf{I}_{(ll)}^{(nn')}\}. \end{aligned} \tag{5.30}$$

We also require the force acting due to a large sphere n', in contact with a small sphere n. The normal component of the displacement for the small sphere, relative to the contact point, is

$$w_{(s)0} = \frac{1}{2}(\mathbf{u}_{(s)}^{(n)} - \mathbf{u}_{(l)}^{(n')}).\mathbf{I}_{(sl)}^{(nn')} \tag{5.31}$$

and the shear component of this relative displacement is thus

$$\frac{1}{2}(\mathbf{u}_{(s)}^{(n)} - \mathbf{u}^{(n')})_{(l)} - [\frac{1}{2}(\mathbf{u}_{(s)}^{(n)} - \mathbf{u}_{(l)}^{(n')}).\mathbf{I}_{(sl)}^{(nn')}]\mathbf{I}_{(sl)}^{(nn')}. \tag{5.32}$$

Also, the normal component of the displacement for the large sphere n' is

$$w_{(l)0} = \frac{1}{2}(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(ls)}^{(n'n)} \tag{5.33}$$

and the shear component

$$\frac{1}{2}(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}^{(n)})_{(s)} - [\frac{1}{2}(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(ls)}^{(n'n)}]\mathbf{I}_{(ls)}^{(n'n)}. \tag{5.34}$$

so that

$$w_{(s)0} + w_{(l)0} = (\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(sl)}^{(nn')}. \tag{5.35}$$

We now have all the information we need to calculate the total force acting on the small sphere n due to its contact with the large sphere n'. From equations (5.9), we thus have

$$\begin{aligned} \mathbf{F}_{(sl)}^{(nn')} &= \frac{(R')^{1/2}}{3\pi B(2B+C)}\{2B[(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(sl)}^{(nn')}]^{1/2}(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(s)}^{(n)} \\ &+(R_l\omega_{(l)}^{(n')} + R_s\omega_{(s)}^{(n)}) \wedge \mathbf{I}_{(sl)}^{(nn')}) + C[(\mathbf{u}_{(l)}^{(n')} - \mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(sl)}^{(nn')}]^{3/2}\mathbf{I}_{(sl)}^{(nn')}\} \end{aligned} \tag{5.36}$$

which can be checked by setting $R_s = R_l$ and comparing with the results of chapter 1. We use this check throughout the work that follows to ensure we are consistent at every stage with the earlier results described.

We need to find an expression for the displacement terms and as a first approximation we again assume that the displacement of each sphere centre is consistent with an applied uniform field and so if the displacement on the boundary is given by

$$u_i = e_{ij}x_j$$

then

$$u_{(s)i}^{(n)} = e_{ij}X_{(s)j}^{(n)}, \tag{5.37}$$

and

$$u_{(l)i}^{(n)} = e_{ij}X_{(l)j}^{(n)}. \tag{5.38}$$

The components of rotation about an axis through the centre of each sphere are

$$\omega_{(s)i}^{(n)} = \omega_{(l)i}^{(n')} = \Omega_i, \tag{5.39}$$

where Ω_i is the average rotation of small and large spheres within the packing. Inserting these into equations (5.29), (5.30) and (5.36) we find

$$\begin{aligned}
F_{(ss)i}^{(nn')} &= -\frac{4R_s^2}{3\pi B(2B+C)}\left\{2B(-e_{pq}I_{(ss)p}^{(nn')}I_{(ss)q}^{(nn')})^{1/2}\left(e_{ij}I_{(ss)j}^{(nn')} - \epsilon_{ijk}\Omega_j I_{(ss)k}^{(nn')}\right)\right. \\
&\qquad \left. -C(-e_{pq}I_{(ss)p}^{(nn')}I_{(ss)q}^{(nn')})^{3/2}I_{(ss)i}^{(nn')}\right\}, \\
F_{(ll)i}^{(nn')} &= -\frac{4R_l^2}{3\pi B(2B+C)}\left\{2B(-e_{pq}I_{(ll)p}^{(nn')}I_{(ll)q}^{(nn')})^{1/2}\left(e_{ij}I_{(ll)j}^{(nn')} - \epsilon_{ijk}\Omega_j I_{(ll)k}^{(nn')}\right)\right. \\
&\qquad \left. -C(-e_{pq}I_{(ll)p}^{(nn')}I_{(ll)q}^{(nn')})^{3/2}I_{(ll)i}^{(nn')}\right\}, \\
F_{(sl)i}^{(nn')} &= -\frac{2(R_lR_s)^{1/2}(R_l+R_s)}{3\pi B(2B+C)}\left\{2B(-e_{pq}I_{(sl)p}^{(nn')}I_{(sl)q}^{(nn')})^{1/2}\left(e_{ij}I_{(sl)j}^{(nn')}\right.\right. \\
&\quad \left.\left. -\epsilon_{ijk}\Omega_j I_{(sl)k}^{(nn')}\right) - C(-e_{pq}I_{(sl)p}^{(nn')}I_{(sl)q}^{(nn')})^{3/2}I_{(sl)i}^{(nn')}\right\}.
\end{aligned} \tag{5.40}$$

For comparison with the work of Jenkins *et al.* [43], we are only concerned with the case of an initial hydrostatic strain. However, for a more complete study we will also discuss the calculations that arise from initial uniaxial and biaxial strains. For a hydrostatic compression the strain takes the form:

$$e_{ij} = e\delta_{ij}, \tag{5.41}$$

with $e < 0$ for compression. For a uniaxial compression it is

$$e_{ij} = e_3\delta_{i3}\delta_{j3} \tag{5.42}$$

with $e_3 < 0$ for compression and for a biaxial compressive strain,

$$e_{ij} = e_1(\delta_{i1}\delta_{j1} + \delta_{i2}\delta_{j2}) + e_3\delta_{i3}\delta_{j3}. \tag{5.43}$$

Hydrostatic Strain

In the case of an initial hydrostatic strain, we use equation (5.41) and the fact that the average rotation term is zero, $\Omega_{(l)i} = \Omega_{(s)i} = 0$. Then equations (5.40), the forces acting on the contact areas reduce to

$$F_{(ss)i}^{(nn')} = \frac{4R_s^2(-e)^{3/2}}{3\pi B}I_{(ss)i}^{(nn')}, \quad F_{(ll)i}^{(nn')} = \frac{4R_l^2(-e)^{3/2}}{3\pi B}I_{(ll)i}^{(nn')} \tag{5.44}$$

and

$$F^{(nn')}_{(sl)i} = \frac{2(R_s R_l)^{1/2}(R_l + R_s)(-e)^{3/2}}{3\pi B} I^{(nn')}_{(sl)i}, \tag{5.45}$$

from which we can calculate the average stress within the medium.

We wish to find an expression for the connection between the average stress within the medium and the average strain. For a random packing of equal sized spheres this is determined from equation (1.88). The analogous general expression for the average stress in the packing of a binary mixture of spheres is given by

$$\begin{aligned} < \sigma_{ij} > \;=\; & -\frac{1}{2V}\{N_s\eta_s R_s(< I_{(ss)i}F_{(ss)j} > + < I_{(ss)j}F_{(ss)i} >) \\ & +N_l\eta_l R_l(< I_{(ll)i}F_{(ll)j} > + < I_{(ll)j}F_{(ll)i} >) \\ & +N_s\eta_{sl} R_s(< I_{(sl)i}F_{(sl)j} > + < I_{(sl)j}F_{(sl)i} >) \\ & +N_l\eta_{ls} R_l(< I_{(ls)i}F_{(ls)j} > + < I_{(ls)j}F_{(ls)i} >)\} \end{aligned} \tag{5.46}$$

in which N_s and N_l are the numbers of small and large spheres in the packing, respectively. Also, η_s, η_l, η_{sl} and η_{ls} are, respectively, the average co-ordination numbers for small-small contacts, large-large contacts, number of large spheres touching a typical small sphere and number of small spheres touching a typical large sphere. The angle brackets on the left hand side of this expression represent a volume average. Those on the right hand side represent average over all contacts in the packing as they have done in previous chapters, but in fact reduce to different sums for each expression. This is clear if we consider $< I_{(ss)i}F_{(ss)j} >$, for example, which will only exist if we were concentrating on the particular contact of one small sphere with another. In this case,

$$< I_{(ss)i}F_{(ss)j} >= \frac{1}{\text{Total Number of Contacts}} \sum_{n\ small} \sum_{n'\ small} I^{(nn')}_{(ss)i} F^{(nn')}_{(ss)j}.$$

Using equations (5.40), the average stress, equation (5.46), is given in general by the following expression:

$$\begin{aligned} < \sigma_{ij} > \;=\; & \frac{2}{3\pi V B(2B+C)}\Big\{B\Big[2N_s\eta_s R_s^3 < (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2}\Big((e_{ik}I_{(ss)k}I_{(ss)j} \\ & +e_{jk}I_{(ss)k}I_{(ss)i}) - (\epsilon_{ikl}\Omega_k I_{(ss)l}I_{(ss)j} + \epsilon_{jkl}\Omega_k I_{(ss)l}I_{(ss)i})\Big) > \\ & +2N_l\eta_l R_l^3 < (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2}\Big((e_{ik}I_{(ll)k}I_{(ll)j} + e_{jk}I_{(ll)k}I_{(ll)i}) \\ & -(\epsilon_{ikl}\Omega_k I_{(ll)l}I_{(ll)j} + \epsilon_{jkl}\Omega_k I_{(ll)l}I_{(ll)i})\Big) > \end{aligned}$$

$$
\begin{aligned}
&+N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 \\
&\qquad < (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2}\Big((e_{ik}I_{(sl)k}I_{(sl)j}+e_{jk}I_{(sl)k}I_{(sl)i}) \\
&-(\epsilon_{ikl}\Omega_kI_{(sl)l}I_{(sl)j}+\epsilon_{jkl}\Omega_kI_{(sl)l}I_{(sl)i}) >\Big] \\
&-C\Big[N_s\eta_sR_s^3 < (-e_{pq}I_{(ss)p}I_{(ss)q})^{3/2}I_{(ss)i}I_{(ss)j} > \\
&\qquad +N_l\eta_lR_l^3 < (-e_{pq}I_{(ll)p}I_{(ll)q})^{3/2}I_{(ll)i}I_{(ll)j} > \\
&+N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 < (-e_{pq}I_{(sl)p}I_{(sl)q})^{3/2}I_{(sl)i}I_{(sl)j} >\Big]\Big\}.
\end{aligned}
\tag{5.47}
$$

Since the angle brackets on the right hand side of this last equation represent the average value over the whole packing then, for example, the values of some typical terms that arise are as follows:

$$
< I_{(ss)i}I_{(ss)j} >= \frac{N_s\eta_s}{3(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij},
$$

$$
< I_{(ll)i}I_{(ll)j} >= \frac{N_l\eta_l}{3(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij},
$$

$$
< I_{(sl)i}I_{(sl)j} >= \frac{N_s\eta_{sl}}{3(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij}.
$$

Thus, in the particular case of an initial hydrostatic strain, $e_{ij}=e\delta_{ij}$, we find that the average stress within the medium is given by:

$$
\begin{aligned}
< \sigma_{ij} > &= -\frac{2(-e)^{3/2}}{3\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2N_l^2R_l^3\eta_l^2 \\
&\qquad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}\delta_{ij}.
\end{aligned}
\tag{5.48}
$$

This is the average stress for the case of infinitely rough spheres, we also consider the result when the spheres are perfectly smooth. The analysis in this second example can be repeated in the same way and as there are now no shear forces acting across the contact area, equation (5.46) reduces to

$$
\begin{aligned}
< \sigma_{ij} > &= -\frac{2}{3\pi VB}\Big\{N_s\eta_sR_s^3 < (-e_{pq}I_{(ss)p}I_{(ss)q})^{3/2}I_{(ss)i}I_{(ss)j} > \\
&\quad +N_l\eta_lR_l^3 < (-e_{pq}I_{(ll)p}I_{(ll)q})^{3/2}I_{(ll)i}I_{(ll)j} > \\
&\quad +N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 < (-e_{pq}I_{(sl)p}I_{(sl)q})^{3/2}I_{(sl)i}I_{(sl)j} >\Big\}
\end{aligned}
\tag{5.49}
$$

Hence, when we apply an initial hydrostatic strain to a packing of perfectly smooth spheres,. the average stress is found to be identical to that for a packing of infinitely rough spheres.

Uniaxial Strain

Now secondly, considering the case of an initial uniaxial strain applied to a packing of infinitely rough spheres we have $e_{ij} = e_3\delta_{i3}\delta_{j3}$ and again find that the rotation terms are zero, $\Omega_{(l)i} = \Omega_{(s)i} = 0$ and the general force equations (5.40) become

$$\begin{aligned} F^{(nn')}_{(ss)i} &= \frac{4R_s^2(-e_3)^{3/2}}{3\pi B(2B+C)}\left\{2B|I^{(nn')}_{(ss)3}|I^{(nn')}_{(ss)3}\delta_{i3} + C|I^{(nn')}_{(ss)3}|^3 I^{(nn')}_{(ss)i}\right\}, \\ F^{(nn')}_{(ll)i} &= \frac{4R_l^2(-e_3)^{3/2}}{3\pi B(2B+C)}\left\{2B|I^{(nn')}_{(ll)3}|I^{(nn')}_{(ll)3}\delta_{i3} + C|I^{(nn')}_{(ll)3}|^3 I^{(nn')}_{(ll)i}\right\} \end{aligned} \tag{5.50}$$

and

$$F^{(nn')}_{(sl)i} = \frac{2(R_sR_l)^{1/2}(R_l+R_s)(-e_3)^{3/2}}{3\pi B(2B+C)}\left\{2B|I^{(nn')}_{(sl)3}|I^{(nn')}_{(sl)3} + C|I^{(nn')}_{(sl)3}|^3 I^{(nn')}_{(sl)3}\right\}. \tag{5.51}$$

To calculate the initial average stress from these we use equation (5.46). We also need the following expressions which arise in the calculation:

$$\begin{aligned} &< |I_{(ss)3}|I_{(ss)3}I_{(ss)j} >= \frac{N_s\eta_s}{4(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{j3} \\ &< |I_{(ll)3}|I_{(ll)3}I_{(ll)j} >= \frac{N_l\eta_l}{4(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{j3} \\ &< |I_{(sl)3}|I_{(sl)3}I_{(sl)j} >= \frac{N_s\eta_{sl}}{4(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{j3} \end{aligned} \tag{5.52}$$

and

$$\begin{aligned} &< |I_{(ss)3}|^3 I_{(ss)i}I_{(ss)j} >= \frac{N_s\eta_s}{(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{\frac{1}{24}\delta_{ij} + \frac{1}{8}\delta_{i3}\delta_{j3}\right\} \\ &< |I_{(ll)i}|^3 I_{(ll)i}I_{(ll)j} >= \frac{N_l\eta_l}{(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{\frac{1}{24}\delta_{ij} + \frac{1}{8}\delta_{i3}\delta_{j3}\right\} \\ &< |I_{(sl)i}|^3 I_{(sl)i}I_{(sl)j} > = \frac{N_s\eta_{sl}}{(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{\frac{1}{24}\delta_{ij} + \frac{1}{8}\delta_{i3}\delta_{j3}\right\}. \end{aligned} \tag{5.53}$$

These are analogous to the equations (1.100) for equal sized spheres. Then we have the initial average stress due to an initial uniaxial strain given by:

$$\begin{aligned} < \sigma_{ij} > &= -\frac{(-e)^{3/2}}{36\pi V B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\ &\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}(C\delta_{ij}+(12B+3C)\delta_{i3}\delta_{j3}) \end{aligned} \tag{5.54}$$

which corresponds to a stress of the form

$$< \sigma_{ij} >= diag(< \sigma_1 >, < \sigma_1 >, < \sigma_3 >), \tag{5.55}$$

with components

$$\begin{aligned} < \sigma_1 > &= -\frac{C(-e)^{3/2}}{36\pi V B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\ &\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\} \end{aligned}$$

and

$$\begin{aligned} < \sigma_3 > &= -\frac{(3B+C)(-e)^{3/2}}{36\pi V B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\ &\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}. \end{aligned} \tag{5.56}$$

If the spheres were perfectly smooth then as there are no shear forces acting across the contact area, we now have

$$F_{(ss)i}^{(nn')} = \frac{4R_s^2(-e_3)^{3/2}}{3\pi B}\left\{|I_{(ss)3}^{(nn')}|^3 I_{(ss)i}^{(nn')}\right\}, \tag{5.57}$$

$$F_{(ll)i}^{(nn')} = \frac{4R_l^2(-e_3)^{3/2}}{3\pi B}\left\{|I_{(ll)3}^{(nn')}|^3 I_{(ll)i}^{(nn')}\right\} \tag{5.58}$$

and

$$F_{(sl)i}^{(nn')} = \frac{2(R_sR_l)^{1/2}(R_l+R_s)(-e_3)^{3/2}}{3\pi B}\left\{|I_{(sl)3}^{(nn')}|^3 I_{(sl)3}^{(nn')}\right\}. \tag{5.59}$$

This again leads to the following form of the initial average stress:

$$< \sigma_{ij} >= diag(< \sigma_1 >, < \sigma_1 >, < \sigma_3 >), \tag{5.60}$$

but with

$$
\begin{aligned}
<\sigma_1> &= -\frac{(-e)^{3/2}}{36\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\
&\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}
\end{aligned}
$$

and

$$
\begin{aligned}
<\sigma_3> &= -\frac{(-e)^{3/2}}{36\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\
&\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}. \qquad (5.61)
\end{aligned}
$$

Biaxial Strain

Finally, we consider the case of an initial biaxial strain, $e_{ij}=e_1(\delta_{i1}\delta_{j1}+\delta_{i2}\delta_{j2})+e_3\delta_{i3}\delta_{j3}$. For a packing of infinitely rough spheres, the force acting across the contact area on the nth small sphere due to its contact with the n'th small sphere is:

$$
\begin{aligned}
F^{(nn')}_{(ss)i} &= \frac{4R_s^2(-e_1)^{3/2}}{3\pi B(2B+C)}\left\{2B\left[1+\frac{(e_3-e_1)}{e_1}I^2_{(ss)3}\right]^{1/2}\right. \\
&\quad \left. x\left(I_{(ss)i}+\frac{(e_3-e_1)}{e_1}\delta_{i3}I_{(ss)3}\right)-C\left[1+\frac{(e_3-e_1)}{e_1}I^2_{(ss)3}\right]^{3/2}I_{(ss)i}\right\} \\
&\qquad (5.62)
\end{aligned}
$$

and a similar expression holds for the force acting on the nth large due to its contact with the n'th large. Rotations are again zero for the initial part of the problem and hence do not appear in these expressions. For the nth small sphere in contact with the n'th large the force acting is:

$$
\begin{aligned}
F^{(nn')}_{(sl)i} &= \frac{(R_sR_l)^{1/2}(R_s+R_l)(-e_1)^{3/2}}{3\pi B(2B+C)}\left\{2B\left[1+\frac{(e_3-e_1)}{e_1}I^2_{(sl)3}\right]^{1/2}\right. \\
&\quad \left. x\left(I_{(sl)i}+\frac{(e_3-e_1)}{e_1}\delta_{i3}I_{(sl)3}\right)-C\left[1+\frac{(e_3-e_1)}{e_1}I^2_{(sl)3}\right]^{3/2}I_{(sl)i}\right\}. \\
&\qquad (5.63)
\end{aligned}
$$

Calculating the initial average stress from these force expressions, we must reintroduce the functions f_1, f_2 and f_3, met in Chapter 2. These are defined as:

$$f_1(x) = \begin{cases} x^{1/2} + \frac{1}{(1-x)^{1/2}} \sin^{-1}(1-x)^{1/2} & \text{if } x < 1 \\ 2 & \text{if } x = 1 \\ x^{1/2} + \frac{1}{(x-1)^{1/2}} \sinh^{-1}(x-1)^{1/2} & \text{if } x > 1 \end{cases} \tag{5.64}$$

$$f_2(x) = \begin{cases} \frac{x^{1/2}(1-2x)}{4(1-x)} + \frac{1}{4(1-x)^{3/2}} \sin^{-1}(1-x)^{1/2} & \text{if } x < 1 \\ 2/3 & \text{if } x = 1 \\ \frac{x^{1/2}(2x-1)}{4(x-1)} - \frac{1}{4(x-1)^{3/2}} \sinh^{-1}(x-1)^{1/2} & \text{if } x > 1 \end{cases} \tag{5.65}$$

$$f_3(x) = \begin{cases} \frac{x^{1/2}(3-2x)}{4(1-x)} + \frac{(3-4x)}{4(1-x)^{3/2}} \sin^{-1}(1-x)^{1/2} & \text{if } x < 1 \\ 4/3 & \text{if } x = 1 \\ \frac{x^{1/2}(2x-3)}{4(x-1)} + \frac{(4x-3)}{4(x-1)^{3/2}} \sinh^{-1}(x-1)^{1/2} & \text{if } x > 1. \end{cases} \tag{5.66}$$

Then the average stress is found to have the form:

$$< \sigma_{ij} >= diag(< \sigma_1 >, < \sigma_1 >, < \sigma_3 >), \tag{5.67}$$

with

$$\begin{aligned} < \sigma_1 > \;=\; & -\frac{(-e_1)^{3/2}}{6\pi VB(2B+C)(N_s(\eta_s+\eta_{sl}) + N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2 \\ & +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2)\} \\ & \left\{(2B+\frac{3C}{4})f_1\left(\frac{e_3}{e_1}\right) - (2B+\frac{C}{2})f_2\left(\frac{e_3}{e_1}\right) + \frac{C}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\} \end{aligned}$$

and

$$\begin{aligned} < \sigma_3 > \;=\; & -\frac{2(-e_1)^{3/2}}{3\pi VB(N_s(\eta_s+\eta_{sl}) + N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2 \\ & +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2)\} \\ & \left\{(\frac{Be_3}{e_1}+\frac{C}{4})f_2\left(\frac{e_3}{e_1}\right) + \frac{C}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\}. \end{aligned} \tag{5.68}$$

These expressions relate to infinitely rough spheres, for a packing of perfectly smooth spheres, we find that the average stress again takes the form of equation (5.67), but with components as follows:

$$
\begin{aligned}
<\sigma_1> &= -\frac{(-e_1)^{3/2}}{6\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2\\
&\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}\\
&\quad x\left\{\frac{3}{4}f_1\left(\frac{e_3}{e_1}\right)-\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\},
\end{aligned}
$$

and

$$
\begin{aligned}
<\sigma_3> &= -\frac{2(-e_1)^{3/2}}{3\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2\\
&\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}\\
&\quad x\left\{\frac{1}{4}f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{6}\left(\frac{e_3}{e_1}\right)^{3/2}\right\}.
\end{aligned}
\tag{5.69}
$$

We can roughly check the validity of all of the expressions found in this chapter by assuming that the spheres are all the same size. This results in the same expressions as found in Walton [86], for the initial hydrostatic and uniaxial strains and those for the initial biaxial strain, found in Chapter 2 of this thesis.

5.3 The Incremental Problem

The second stage in the calculation of the effective elastic moduli is to apply an additional incremental displacement to the boundary. Further to the initial state, we have a displacement of the boundary $\delta\mathbf{u}$ and this is consistent with a uniform strain, δe_{ij} and so

$$\delta u_i = \delta e_{ij}x_j. \tag{5.70}$$

The centre of the nth sphere will also undergo a further displacement $\delta\mathbf{u}^{(n)}$. Considering a packing of infinitely rough spheres first, we calculate the incremental force acting on the nth sphere due to its contact with the n'th sphere. If the nth and n' th spheres are both small we have

$$
\begin{aligned}
\delta\mathbf{F}_{(ss)}^{(nn')} &= \frac{(2R_s)^{1/2}[(\mathbf{u}_{(s)}^{(n')}-\mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(ss)}^{(nn')}]^{1/2}}{2\pi B(2B+C)}\Big\{2B(\delta\mathbf{u}_{(s)}^{(n')}-\delta\mathbf{u}_{(s)}^{(n)}\\
&\quad +R_s\epsilon_{ijk}(\delta\omega_{(s)}^{(n')}+\delta\omega_{(s)}^{(n)})\mathbf{I}_{(ss)}^{(nn')})+C[(\delta\mathbf{u}_{(s)}^{(n')}-\delta\mathbf{u}_{(s)}^{(n)}).\mathbf{I}_{(ss)}^{(nn')}]\mathbf{I}_{(ss)}^{(nn')}\Big\}.
\end{aligned}
\tag{5.71}
$$

Similarly, the force acting on a large sphere n due to its contact with another large sphere n' is:

$$\begin{aligned}\delta\mathbf{F}^{(nn')}_{(ll)} &= \frac{(2R_s)^{1/2}[(\mathbf{u}^{(n')}_{(l)} - \mathbf{u}^{(n)}_{(l)}).\mathbf{I}^{(nn')}_{(ll)}]^{1/2}}{2\pi B(2B+C)}\Big\{2B(\delta\mathbf{u}^{(n')}_{(l)} - \delta\mathbf{u}^{(n)}_{(l)} \\ &+R_s\epsilon_{ijk}(\delta\omega^{(n')}_{(l)} + \delta\omega^{(n)}_{(l)})\mathbf{I}^{(nn')}_{(ll)}) + C[(\delta\mathbf{u}^{(n')}_{(l)} - \delta\mathbf{u}^{(n)}_{(l)})).\mathbf{I}^{(nn')}_{(ll)}]\mathbf{I}^{(nn')}_{(ll)}\Big\}.\end{aligned} \tag{5.72}$$

Also, the force acting on a small sphere due to its contact with a large is:

$$\begin{aligned}\delta\mathbf{F}^{(nn')}_{(sl)} &= \frac{2(R')^{1/2}[(\mathbf{u}^{(n')}_{(l)} - \mathbf{u}^{(n)}_{(s)}).\mathbf{I}^{(nn')}_{(sl)}]^{1/2}}{2\pi B(2B+C)}\Big\{2B(\delta\mathbf{u}^{(n')}_{(l)} - \delta\mathbf{u}^{(n)}_{(s)} \\ &+R_s\epsilon_{ijk}(\delta\omega^{(n')}_{(l)} + \delta\omega^{(n)}_{(s)})\mathbf{I}^{(nn')}_{(sl)}) + C[(\delta\mathbf{u}^{(n')}_{(l)} - \delta\mathbf{u}^{(n)}_{(s)})).\mathbf{I}^{(nn')}_{(sl)}]\mathbf{I}^{(nn')}_{(sl)}\Big\}.\end{aligned} \tag{5.73}$$

As a first approximation, we assume that the displacement of the centre of the nth sphere is again given by the uniform strain approximation for the incremental case. That is, assume that the centre of the nth sphere is displaced by

$$\delta u^{(n)}_{(s)i} = \delta e_{ij}X^{(n)}_{(s)j},$$

$$\delta u^{(n)}_{(l)i} = \delta e_{ij}X^{(n)}_{(l)j},$$

for the nth sphere small or large respectively and

$$\delta\omega^{(n)}_{(s)i} = \delta\omega^{(n)}_{(l)i} = \delta\Omega_i.$$

This gives the incremental force acting on the nth small sphere, due to its contact with the n'th small sphere as

$$\begin{aligned}\delta F^{(nn')}_{(ss)i} &= -\frac{2R_s^2(-e_{pq}I^{(nn')}_{(ss)p}I^{(nn')}_{(ss)q})^{1/2}}{\pi B(2B+C)}\{2B(\delta e_{ik}I^{(nn')}_{(ss)k} + \epsilon_{ikj}\delta\omega_j I_{(ss)k}) \\ &+C\delta e_{kl}I^{(nn')}_{(ss)k}I^{(nn')}_{(ss)l}I^{(nn')}_{(ss)i}\}\end{aligned} \tag{5.74}$$

and again a similar expression for the force acting on a large sphere n due to its contact with a large sphere n' is found. The force acting on a small sphere due to its contact with a large is given by:

$$\delta F^{(nn')}_{(sl)i} = -\frac{(R_sR_l)^{1/2}(R_l+R_s)(-e_{pq}I^{(nn')}_{(sl)p}I^{(nn')}_{(sl)q})^{1/2}}{\pi B(2B+C)}\{2B(\delta e_{ik}I^{(nn')}_{(sl)k} + \epsilon_{ikj}\delta\omega_j I_{(sl)k}) + C\delta e_{kl}I^{(nn')}_{(sl)k}I^{(nn')}_{(sl)l}I^{(nn')}_{(sl)i}\}. \tag{5.75}$$

In chapter 1, we discussed the work done by Slade [76] to include the effects of sphere rotations upon the moduli. Here we must consider the equivalent equations of equilibrium, those of the forces and moments acting on each individual sphere. The general condition that arose from the equilibrium of moments upon consideration of equal sized spheres and which had to be satisfied by the rotations was given in equation (1.149) as

$$< (-e_{pq}I_pI_q)^{1/2}(\delta_{ik}-I_iI_k) >< \delta\omega_k >=< \epsilon_{irk}(-e_{pq}I_pI_q)^{1/2}I_rI_l >< \delta e_{kl} > . \tag{5.76}$$

We find that the two analogous expressions for our binary packing of spheres are, firstly from the equilibrium of moments acting on the nth small sphere,

$$\begin{aligned}2R_s^2 \Big(\epsilon_{irk} &< (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2}I_{(ss)r}I_{(ss)l} >< \delta e_{kl} > \\ &+ < (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2}(\delta_{ik}-I_{(ss)i}I_{(ss)k}) >< \delta\omega_k >\Big) \\ = (R_sR_l)^{1/2}(R_l+R_s)\Big(\epsilon_{irk} &< (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2}I_{(sl)r}I_{(sl)l} >< \delta e_{kl} > \\ &+ < (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2}(\delta_{ik}-I_{(sl)i}I_{(sl)k}) >< \delta\omega_k >\Big)\end{aligned} \tag{5.77}$$

and second, that from equilibrium of moments of the nth large sphere

$$\begin{aligned}2R_l^2 \Big(\epsilon_{irk} &< (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2}I_{(ll)r}I_{(ll)l} >< \delta e_{kl} > \\ &+ < (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2}(\delta_{ik}-I_{(ll)i}I_{(ll)k}) >< \delta\omega_k >\Big) \\ = (R_sR_l)^{1/2}(R_l+R_s)\Big(&< \epsilon_{irk}(-e_{pq}I_{(ls)p}I_{(ls)q})^{1/2}I_{(ls)r}I_{(ls)l} >< \delta e_{kl} > \\ &+ < (-e_{pq}I_{(ls)p}I_{(ls)q})^{1/2}(\delta_{ik}-I_{(ls)i}I_{(ls)k}) >< \delta\omega_k >\Big).\end{aligned} \tag{5.78}$$

These allow us to calculate the components of the rotation for each sphere.

Initial Hydrostatic Compression

Considering first the case of an initial hydrostatic strain, $e_{ij} = e\delta_{ij}$, we find from the equations above that the incremental rotation term $\delta\omega_i$ is zero and then the forces acting across the contact area are given by:

$$\delta F^{(nn')}_{(ss)i} = \frac{-2R_s^2(-e)^{1/2}}{\pi B(2B+C)}\left\{2B\delta e_{ij}I^{(nn')}_{(ss)j} + C\delta e_{kl}I^{(nn')}_{(ss)k}I^{(nn')}_{(ss)l}I^{(nn')}_{(ss)i}\right\} \tag{5.79}$$

and similarly,

$$\delta F^{(nn')}_{(ll)i} = \frac{-2R_l^2(-e)^{1/2}}{\pi B(2B+C)}\left\{2B\delta e_{ij}I^{(nn')}_{(ll)j} + C\delta e_{kl}I^{(nn')}_{(ll)k}I^{(nn')}_{(ll)l}I^{(nn')}_{(ll)i}\right\}. \tag{5.80}$$

Also,

$$\delta F^{(nn')}_{(sl)i} = \frac{-(R_sR_l)^{1/2}(R_s+R_l)(-e)^{1/2}}{\pi B(2B+C)}\left\{2B\delta e_{ij}I^{(nn')}_{(sl)j} + C\delta e_{kl}I^{(nn')}_{(sl)k}I^{(nn')}_{(sl)l}I^{(nn')}_{(sl)i}\right\}. \tag{5.81}$$

From these expressions, we calculate the average incremental stress using a similar equation to (5.46), that is

$$\begin{aligned} < \delta\sigma_{ij} > \;=\; & -\frac{1}{2V}\{N_s\eta_sR_s(< I_{(ss)i}\delta F_{(ss)j} > + < I_{(ss)j}\delta F_{(ss)i} >) \\ & +N_l\eta_lR_l(< I_{(ll)i}\delta F_{(ll)j} > + < I_{(ll)j}\delta F_{(ll)i} >) \\ & +N_s\eta_{sl}R_s(< I_{(sl)i}\delta F_{(sl)j} > + < I_{(sl)j}\delta F_{(sl)i} >) \\ & +N_l\eta_{ls}R_l(< I_{(ls)i}\delta F_{(ls)j} > + < I_{(ls)j}\delta F_{(ls)i} >)\}, \end{aligned} \tag{5.82}$$

which in the general case amounts to:

$$\begin{aligned} < \delta\sigma_{ij} > \;=\; & \frac{2}{3\pi VB(2B+C)}\Big\{B\Big[2N_s\eta_sR_s^3 < (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2}\Big((\delta e_{ik}I_{(ss)k}I_{(ss)j} \\ & +\delta e_{jk}I_{(ss)k}I_{(ss)i}) - (\epsilon_{ikl}\delta\Omega_kI_{(ss)l}I_{(ss)j} + \epsilon_{jkl}\delta\Omega_kI_{(ss)l}I_{(ss)i})\Big) > \\ & +2N_l\eta_lR_l^3 < (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2}\Big((\delta e_{ik}I_{(ll)k}I_{(ll)j} + \delta e_{jk}I_{(ll)k}I_{(ll)i}) \\ & -(\epsilon_{ikl}\delta\Omega_kI_{(ll)l}I_{(ll)j} + \epsilon_{jkl}\delta\Omega_kI_{(ll)l}I_{(ll)i})\Big) > \\ & +N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 \\ & < (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2}\Big((\delta e_{ik}I_{(sl)k}I_{(sl)j} + \delta e_{jk}I_{(sl)k}I_{(sl)i}) \\ & +(\epsilon_{ikl}\delta\Omega_kI_{(sl)l}I_{(sl)j} + \epsilon_{jkl}\delta\Omega_kI_{(sl)l}I_{(sl)i}) >\Big] \end{aligned}$$

$$+C\Big[2N_s\eta_s R_s^3 < (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2}I_{(ss)i}I_{(ss)j}I_{(ss)k}I_{(ss)l} >< \delta e_{kl} >$$
$$+2N_l\eta_l R_l^3 < (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2}I_{(ll)i}I_{(ll)j}I_{(ss)k}I_{(ss)l} >< \delta e_{kl} >$$
$$+N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2$$
$$< (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2}I_{(sl)i}I_{(sl)j}I_{(ss)k}I_{(ss)l}\delta e_{kl} >\Big]\Big\}. \tag{5.83}$$

This enables us to relate the average incremental stress to the average incremental strain and this is what is required to compute the effective moduli.

Using the fact that

$$< I_{(ss)i}I_{(ss)j} >= \frac{N_s\eta_s}{3(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij},$$

$$< I_{(ll)i}I_{(ll)j} >= \frac{N_l\eta_l}{3(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij},$$
$$< I_{(sl)i}I_{(sl)j} >= \frac{N_s\eta_{sl}}{3(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij}$$

and also

$$< I_{(ss)i}I_{(ss)j}I_{(ss)k}I_{(ss)k} >= \frac{N_s\eta_s}{15(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij},$$

$$< I_{(ll)i}I_{(ll)j}I_{(ll)k}I_{(ll)k} >= \frac{N_l\eta_l}{15(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij},$$
$$< I_{(sl)i}I_{(sl)j}I_{(sl)k}I_{(sl)k} >= \frac{N_s\eta_{sl}}{15(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\delta_{ij},$$

we can now calculate this stress.

So, for an initial hydrostatic strain we find

$$\begin{aligned} < \delta\sigma_{ij} > \;=\; & \frac{(-e)^{1/2}}{15\pi VB(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\Big\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\ & +(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})\Big\} \\ & x\{5B(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})+C(\delta_{ij}\delta_{jk}+\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\}. \end{aligned} \tag{5.84}$$

The effective moduli are defined by:

$$< \delta\sigma_{ij} >= C^*_{ijkl} < \delta e_{kl} > \tag{5.85}$$

and thus we can calculate them directly from the average incremental stress. We also note that the general expression for these moduli is found to be:

$$\begin{aligned}
C^*_{ijkl} &= \frac{1}{3\pi VB(2B+C)} \Big\{ B \Big[2N_s\eta_s R_s^3 (< (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2} I_{(ss)k}I_{(ss)j} > \delta_{il} \\
&\qquad + < (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2} I_{(ss)k}I_{(ss)i} > \delta_{jl}) \\
&\quad +2N_l\eta_l R_l^3 (< (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2} I_{(ll)k}I_{(ll)j} > \delta_{il} \\
&\qquad + < (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2} I_{(ll)k}I_{(ll)i} > \delta_{jl}) \\
&\quad +N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 (< (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2} I_{(sl)k}I_{(sl)j} > \delta_{il} \\
&\qquad + < (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2} I_{(sl)k}I_{(sl)i} > \delta_{jl}) \Big] \\
&\quad +2C \Big[N_s\eta_s R_s^3 (< (-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2} I_{(ss)i}I_{(ss)j}I_{(ss)k}I_{(ss)l} > \\
&\quad +N_l\eta_l R_l^3 < (-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2} I_{(ll)i}I_{(ll)j}I_{(ll)k}I_{(ll)l} > \\
&\quad +N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 < (-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2} I_{(sl)i}I_{(sl)j}I_{(sl)k}I_{(sl)l} > \Big] \Big\},
\end{aligned} \tag{5.86}$$

which is the analogue of equation (1.111) in Chapter 1. This latter equation gives the general expression for the moduli when the spheres are equal in size, provided rotation components are zero, as they are in the hydrostatic case.

Returning to our case of initial compression then, the hydrostatic case. Equation (5.86) reduces to:

$$\begin{aligned}
C^*_{ijkl} &= \frac{(-e)^{1/2}}{3\pi VB(2B+C)} \Big\{ B \Big[2N_s\eta_s R_s^3 (< I_{(ss)k}I_{(ss)j} > \delta_{il} \\
&\qquad + < I_{(ss)k}I_{(ss)i} > \delta_{jl}) \\
&\quad +2N_l\eta_l R_l^3 (< I_{(ll)k}I_{(ll)j} > \delta_{il} + < I_{(ll)k}I_{(ll)i} > \delta_{jl}) \\
&\quad +N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 (< I_{(sl)k}I_{(sl)j} > \delta_{il} + < I_{(sl)k}I_{(sl)i} > \delta_{jl}) \Big] \\
&\quad +2C \Big[N_s\eta_s R_s^3 (< I_{(ss)i}I_{(ss)j}I_{(ss)k}I_{(ss)l} > +N_l\eta_l R_l^3 < I_{(ll)i}I_{(ll)j}I_{(ll)k}I_{(ll)l} > \\
&\quad +N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 < I_{(sl)i}I_{(sl)j}I_{(sl)k}I_{(sl)l} > \Big] \Big\},
\end{aligned} \tag{5.87}$$

and so

$$C^*_{ijkl} = \lambda^*\delta_{ij}\delta_{kl} + \mu^*(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \tag{5.88}$$

where the effective Lamé moduli are

$$\begin{aligned}\lambda^* &= \frac{(-e)^{1/2}C}{15\pi VB(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2N_s^2\eta_s^2R_s^3 \\ &\quad +2N_l^2\eta_l^2R_l^3+(R_sR_l)^{1/2}(R_s+R_l)(N_s^2\eta_{sl}^2R_s+N_l^2\eta_{ls}^2R_l)\}\end{aligned} \tag{5.89}$$

and

$$\begin{aligned}\mu^* &= \frac{(-e)^{1/2}(5B+C)}{15\pi VB(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2N_s^2\eta_s^2R_s^3 \\ &\quad +2N_l^2\eta_l^2R_l^3+(R_sR_l)^{1/2}(R_s+R_l)(N_s^2\eta_{sl}^2R_s+N_l^2\eta_{ls}^2R_l)\}.\end{aligned} \tag{5.90}$$

We can also calculate the effective bulk modulus from these which is given by:

$$\begin{aligned}\kappa^* &= \lambda^* + \frac{2}{3}\mu^* \\ &= \frac{(-e)^{1/2}}{3\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\ &\quad +(R_lR_s)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}.\end{aligned} \tag{5.91}$$

The above expressions all relate to a packing of infinitely rough spheres. If we now consider a packing of perfectly smooth spheres, we find that the average incremental stress in the general case is

$$\begin{aligned}<\delta\sigma_{ij}> &= \frac{2}{3\pi VB}\Big\{N_s\eta_sR_s^3<(-e_{pq}I_{(ss)p}I_{(ss)q})^{1/2}I_{(ss)i}I_{(ss)j}I_{(ss)k}I_{(ss)l}><\delta e_{kl}> \\ &\quad +N_l\eta_lR_l^3<(-e_{pq}I_{(ll)p}I_{(ll)q})^{1/2}I_{(ll)i}I_{(ll)j}I_{(ss)k}I_{(ss)l}><\delta e_{kl}> \\ &\quad +N_s\eta_{sl}(R_lR_s)^{1/2}(R_s+R_l)^2 \\ &\qquad <(-e_{pq}I_{(sl)p}I_{(sl)q})^{1/2}I_{(sl)i}I_{(sl)j}I_{(ss)k}I_{(ss)l}><\delta e_{kl}>\Big\}.\end{aligned} \tag{5.92}$$

For an initial hydrostatic strain, the effective moduli are then found to be

$$\begin{aligned}\lambda^*=\mu^* &= \frac{(-e)^{1/2}}{15\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2N_s^2\eta_s^2R_s^3 \\ &\quad +2N_l^2\eta_l^2R_l^3+(R_sR_l)^{1/2}(R_s+R_l)(N_s^2\eta_{sl}^2R_s+N_l^2\eta_{ls}^2R_l)\}\end{aligned} \tag{5.93}$$

and κ^* the effective bulk modulus, is the same as that for the infinitely rough packing, see equation (5.91).

Initial Uniaxial Compression

Turning now to another of our initial conditions, that of an uniaxial compression, using equations (5.77) and (5.78), we can determine expressions for the rotations that occur for the individual spheres. Substituting for the strain $e_{ij} = e_3\delta_{i3}\delta_{j3}$, initially in equation (5.77), we find the components of $\delta\omega_i$. These are given by:

$$\begin{aligned}\delta\omega_1 &= -\frac{1}{3}\delta e_{23}\\ \delta\omega_2 &= \frac{1}{3}\delta e_{13}\end{aligned}\tag{5.94}$$

and

$$\delta\omega_3 = 0.\tag{5.95}$$

In fact these are identical to those found for a packing of equal sized spheres $R_s = R_l$ and are independent of the radii of the spheres.

We can now proceed to calculate the forces acting across the contact area. We have

$$\begin{aligned}\delta F_{(ss)i} &= -\frac{2R_s^2(-e_3)^{1/2}}{\pi B(2B+C)}\Big\{2B(\delta e_{ik}|I_{(ss)3}|I_{(ss)k} - \epsilon_{ijk}\delta\omega_j|I_{(ss)3}|I_{(ss)k})\\ &\quad +C\delta e_{kl}|I_{(ss)3}|I_{(ss)k}I_{(ss)l}I_{(ss)i}\Big\},\end{aligned}\tag{5.96}$$

$$\begin{aligned}\delta F_{(ll)i} &= -\frac{2R_l^2(-e_3)^{1/2}}{\pi B(2B+C)}\Big\{2B(\delta e_{ik}|I_{(ll)3}|I_{(ll)k} - \epsilon_{ijk}\delta\omega_j|I_{(ll)3}|I_{(ll)k})\\ &\quad +C\delta e_{kl}|I_{(ll)3}|I_{(ll)k}I_{(ll)l}I_{(ll)i}\Big\}\end{aligned}\tag{5.97}$$

and

$$\begin{aligned}\delta F_{(sl)i} &= -\frac{(R_sR_l)^{1/2}(R_l+R_s)(-e_3)^{1/2}}{\pi B(2B+C)}\Big\{2B(\delta e_{ik}|I_{(sl)3}|I_{(sl)k}\\ &\quad -\epsilon_{ijk}\delta\omega_j|I_{(sl)3}|I_{(sl)k}) + C\delta e_{kl}|I_{(sl)3}|I_{(sl)k}I_{(sl)l}I_{(sl)i}\Big\}.\end{aligned}\tag{5.98}$$

These allow us to calculate the average incremental stress. We need the average values found in equations (5.52) and (5.53) and also some further expressions:

$$< |I_{(ss)3}| I^2_{(ss)1} >= \frac{N_s\eta_s}{8(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(ss)3}| I^2_{(ss)1} I^2_{(ss)2} >= \frac{N_s\eta_s}{48(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(ss)3}| I^4_{(ss)1} >= \frac{N_s\eta_s}{16(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(ll)3}| I^2_{(ll)1} >= \frac{N_l\eta_l}{8(N_l(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(ll)3}| I^2_{(ll)1} I^2_{(ll)2} >= \frac{N_l\eta_l}{48(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(ll)3}| I^4_{(ll)1} >= \frac{N_l\eta_l}{16(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(sl)3}| I^2_{(sl)1} >= \frac{N_s\eta_{sl}}{8(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(sl)3}| I^2_{(sl)1} I^2_{(sl)2} >= \frac{N_s\eta_{sl}}{48(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))},$$

$$< |I_{(sl)3}| I^4_{(sl)1} >= \frac{N_s\eta_{sl}}{16(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}. \tag{5.99}$$

We note further that,

$$\epsilon_{jpq} < |I_{(ss)3}| I_{(ss)i} I_{(ss)q} >= \epsilon_{jpq} < |I_{(ll)3}| I_{(ll)i} I_{(ll)q} >= \epsilon_{jpq} < |I_{(sl)3}| I_{(sl)i} I_{(sl)q} >= 0, \tag{5.100}$$

if $i = j$ and so rotations will not effect the components $< \delta\sigma_{11} >=< \delta\sigma_{22} >$ and $< \delta\sigma_{33} >$, of the average incremental stress. Hence, rotation term effects will only occur in the modulus C^*_{1313}, as we would expect for consistency with Slade's results [76], for equal sized spheres.

Now, combining all these results, we find the average incremental stress. In particular,

$$\begin{aligned} < \delta\sigma_{11} > \; = \; & \frac{(-e)^{1/2}}{48V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \big\{ 2R_s^3 N_s^2 \eta_s^2 \\ & +2R_l^3 N_l^2 \eta_l^2 + (R_s N_s \eta_{sl} + R_l N_l \eta_{ls})(R_s R_l)^{1/2}(R_s+R_l) \big\} \\ & (12B < \delta e_{11} > + C(\delta kl + 2\delta_{k1}\delta_{l1}) < \delta e_{kl} >), \end{aligned} \tag{5.101}$$

which allows us to calculate the three moduli:

$$\begin{aligned}
C^*_{1111} &= \frac{(4B+C)(-e)^{1/2}}{16V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\
&\quad \left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\}, \\
C^*_{1122} &= \frac{C(-e)^{1/2}}{48V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\
&\quad \left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\}, \\
C^*_{1133} &= \frac{C(-e)^{1/2}}{24V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\
&\quad \left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\} \\
&= 2C^*_{1122}. \qquad (5.102)
\end{aligned}$$

Also,

$$\begin{aligned}
<\delta\sigma_{33}> &= \frac{(-e)^{1/2}}{24V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{2R_s^3N_s^2\eta_s^2\right. \\
&\quad \left.+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(R_s+R_l)\right\} \\
&\quad (12B<\delta e_{33}>+C(\delta kl+3\delta_{k1}\delta_{l1})<\delta e_{kl}>), \qquad (5.103)
\end{aligned}$$

from which we find

$$\begin{aligned}
C^*_{3333} &= \frac{(3B+C)(-e)^{1/2}}{6V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})}+N_l(\eta_l+\eta_{ls})) \\
&\quad \left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\}. \qquad (5.104)
\end{aligned}$$

To find the last modulus we consider $<\delta\sigma_{13}>$, which does involve the rotation terms. Recalling from equation (5.94) and (5.95), the rotation terms, we have

$$\begin{aligned}
<\delta\sigma_{13}> &= \frac{(-e)^{1/2}(4B+C)}{12V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{(2R_s^3N_s^2\eta_s^2\right. \\
&\quad \left.+2R_l^3N_l^2\eta_l^2+(R_sR_l)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\right\}. \qquad (5.105)
\end{aligned}$$

The fifth effective elastic modulus is found to be

$$\begin{aligned}
C^*_{1313} &= \frac{(-e)^{1/2}(4B+C)}{24V\pi B(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{(2R_s^3N_s^2\eta_s^2\right. \\
&\quad \left.+2R_l^3N_l^2\eta_l^2+(R_sR_l)^{1/2}(R_l+R_s)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\right\}. \qquad (5.106)
\end{aligned}$$

We thus have our five independent elastic moduli and each has been checked by comparing with the moduli for a packing of equal sized spheres.

We have considered a packing of infinitely rough spheres, but we can again also consider the effective moduli for a packing of perfectly smooth spheres. We find the average incremental stress, in order to calculate the moduli:

$$\begin{aligned} < \delta\sigma_{11} > &= \frac{(-e)^{1/2}}{48V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2\right. \\ &\left.+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(R_s+R_l)\right\}(\delta kl+2\delta_{k1}\delta_{l1}) < \delta e_{kl} >, \end{aligned} \tag{5.107}$$

from which we have

$$\begin{aligned} C^*_{1111} &= \frac{(-e)^{1/2}}{16V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\ &\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\}, \\ C^*_{1122} &= \frac{(-e)^{1/2}}{48V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\ &\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\}, \\ C^*_{1133} &= \frac{(-e)^{1/2}}{24V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\ &\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\} \\ &= 2C^*_{1122}. \end{aligned} \tag{5.108}$$

Also

$$\begin{aligned} < \delta\sigma_{33} > &= \frac{(-e)^{1/2}}{24V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2\right. \\ &\left.+(R_sN_s^2\eta_{sl}^2+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(R_s+R_l)\right\}(\delta kl+3\delta_{k1}\delta_{l1}) < \delta e_{kl} > \end{aligned} \tag{5.109}$$

and so

$$\begin{aligned} C^*_{3333} &= \frac{(-e)^{1/2}}{6V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\ &\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\}. \end{aligned} \tag{5.110}$$

The final modulus is again found from $< \delta\sigma_{13} >$:

$$
\begin{aligned}
< \delta\sigma_{13} > &= \frac{(-e)^{1/2}}{12V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\left\{(2R_s^3N_s^2\eta_s^2\right. \\
&\left. +2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2})\right\} < \delta e_{13} > . \quad (5.111)
\end{aligned}
$$

and is given by

$$
\begin{aligned}
C^*_{1313} &= \frac{(-e)^{1/2}}{48V\pi B(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\
&\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right\}. \\
& \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad (5.112)
\end{aligned}
$$

Thus, we have our five independent elastic moduli and these too can be checked by comparing with the moduli for a packing of equal sized spheres.

Initial Biaxial Compression

We must also consider the effects of rotation when we have an initial biaxial compression. Again using equations (5.77) and (5.78), we can find expressions for the rotations of the individual spheres. Substituting in the initial strain to equation (5.77), we find an expression for $\delta\omega$ from which, using equation (5.78), we find the components of rotation for a typical sphere are given by:

$$
\begin{aligned}
\delta\omega_1 &= \left(\frac{f_3\left(\frac{e_3}{e_1}\right)-2f_2\left(\frac{e_3}{e_1}\right)}{2f_1\left(\frac{e_3}{e_1}\right)-f_3\left(\frac{e_3}{e_1}\right)}\right)\delta e_{23}, \\
\delta\omega_2 &= \left(\frac{2f_2\left(\frac{e_3}{e_1}\right)-f_3\left(\frac{e_3}{e_1}\right)}{2f_1\left(\frac{e_3}{e_1}\right)-f_3\left(\frac{e_3}{e_1}\right)}\right)\delta e_{13} \qquad (5.113)
\end{aligned}
$$

and

$$\delta\omega_3 = 0. \qquad (5.114)$$

Similarly to the expressions for an initial uniaxial strain, these expressions are identical to those for a packing of equal sized spheres and are independent of the sphere radii. To find the effective moduli we must now calculate the incremental average stress.

The general expression for the average incremental stress, $< \delta\sigma_{ij} >$, for this biaxial compression, including individual sphere rotations, is found from the expressions for the incremental forces acting across the contact areas. In fact, the rotations do not affect the components of this stress if $i = j$, this was also the case for the uniaxial compression. We find

$$
\begin{aligned}
<\delta\sigma_{11}> \;=\; & \frac{(-e)^{1/2}}{\pi V B(2B+C)} \Big\{ 2N_s\eta_s R_s^3 \\
& \Big[2B < (1+\frac{e_3-e_1}{e_1} I_{(ss)3}^2)^{1/2} I_{(ss)k} I_{(ss)1} >< \delta e_{k1} > \\
& \quad + C < (1+\frac{e_3-e_1}{e_1} I_{(ss)3}^2)^{1/2} I_{(ss)1}^2 I_{(ss)k} I_{(ss)l} >< \delta e_{kl} > \Big] \\
& + 2N_l\eta_l R_l^3 \Big[2B < (1+\frac{e_3-e_1}{e_1} I_{(ll)3}^2)^{1/2} I_{(ll)k} I_{(ll)1} >< \delta e_{k1} > \\
& \quad + C < (1+\frac{e_3-e_1}{e_1} I_{(ll)3}^2)^{1/2} I_{(ll)1}^2 I_{(ll)k} I_{(ll)l} >< \delta e_{kl} > \Big] \\
& + (R_s)^{1/2}(R_s+R_l)(R_sN_s\eta_{sl} + R_lN_l\eta_{ls}) \\
& \quad \Big[2B < (1+\frac{e_3-e_1}{e_1} I_{(sl)3}^2)^{1/2} I_{(sl)k} I_{(sl)1} >< \delta e_{k1} > \\
& \quad + C < (1+\frac{e_3-e_1}{e_1} I_{(sl)3}^2)^{1/2} I_{(sl)1}^2 I_{(sl)k} I_{(sl)l} >< \delta e_{kl} > \Big] \Big\}.
\end{aligned}
\tag{5.115}
$$

From this, we then find the three moduli C^*_{1111}, C^*_{1122} and C^*_{1133}. These are:

$$
\begin{aligned}
C^*_{1111} \;=\; & \frac{(-e_1)^{1/2}}{2\pi V B(2B+C)(N_s(\eta_s+\eta_{sl}) + N_l(\eta_l+\eta_{ls}))} \\
& \left\{ 2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2 (R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2) \right\} \\
& \left\{ Bf_3\left(\frac{e_3}{e_1}\right) + \frac{3}{8}C \left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(\frac{1}{2} - \frac{e_3}{e_1}\right) f_2\left(\frac{e_3}{e_1}\right)}{\frac{e_3}{e_1} - 1} + f_3\left(\frac{e_3}{e_1}\right) \right] \right\}, \\
C^*_{1122} \;=\; & \frac{C(-e_1)^{1/2}}{16\pi V B(2B+C)(N_s(\eta_s+\eta_{sl}) + N_l(\eta_l+\eta_{ls}))} \\
& \left\{ 2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2 (R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2) \right\} \\
& \left\{ \frac{(\frac{1}{2} - \frac{e_3}{e_1}) f_2\left(\frac{e_3}{e_1}\right) + \frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}}{\frac{e_3}{e_1} - 1} + f_3\left(\frac{e_3}{e_1}\right) \right\},
\end{aligned}
\tag{5.116}
$$

and

$$
\begin{aligned}
C^*_{1133} \;=\; & \frac{C(-e_1)^{1/2}}{4\pi V B(2B+C)(N_s(\eta_s+\eta_{sl}) + N_l(\eta_l+\eta_{ls}))} \\
& \left\{ 2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2 (R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2) \right\}
\end{aligned}
$$

$$\left\{\frac{\left(\frac{e_3}{e_1}\right)-\frac{1}{2})f_2\left(\frac{e_3}{e_1}\right)-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}}{\frac{e_3}{e_1}-1}\right\}. \tag{5.117}$$

We also have

$$\begin{aligned}
<\delta\sigma_{33}> &= \frac{(-e)^{1/2}}{\pi VB(2B+C)}\left\{2N_s\eta_s R_s^3\right.\\
&\left[2B<(1+\frac{e_3-e_1}{e_1}I_{(ss)3}^2)^{1/2}I_{(ss)k}I_{(ss)3}><\delta e_{k3}>\right.\\
&\left.+C<(1+\frac{e_3-e_1}{e_1}I_{(ss)3}^2)^{1/2}I_{(ss)3}^2I_{(ss)k}I_{(ss)l}><\delta e_{kl}>\right]\\
&+2N_l\eta_l R_l^3\left[2B<(1+\frac{e_3-e_1}{e_1}I_{(ll)3}^2)^{1/2}I_{(ll)k}I_{(ll)3}><\delta e_{k3}>\right.\\
&\left.+C<(1+\frac{e_3-e_1}{e_1}I_{(ll)3}^2)^{1/2}I_{(ll)3}^2I_{(ll)k}I_{(ll)l}><\delta e_{kl}>\right]\\
&+(R_s)^{1/2}(R_s+R_l)(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})\\
&\left[2B<(1+\frac{e_3-e_1}{e_1}I_{(sl)3}^2)^{1/2}I_{(sl)k}I_{(sl)3}><\delta e_{k3}>\right.\\
&\left.\left.+C<(1+\frac{e_3-e_1}{e_1}I_{(sl)3}^2)^{1/2}I_{(sl)3}^2I_{(sl)k}I_{(sl)l}><\delta e_{kl}>\right]\right\}.
\end{aligned} \tag{5.118}$$

and hence

$$\begin{aligned}
C^*_{3333} &= \frac{(-e_1)^{1/2}}{2\pi VB(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\\
&\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\right\}\\
&\left\{2Bf_2\left(\frac{e_3}{e_1}\right)+C\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+-\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)}{\frac{e_3}{e_1}-1}\right]\right\}.
\end{aligned} \tag{5.119}$$

Finally, we calculate the fifth independent modulus from $<\delta\sigma_{13}>$ which does include the effects of rotations:

$$\begin{aligned}
<\delta\sigma_{13}> &= \frac{(-e)^{1/2}}{\pi VB(2B+C)}\left\{2N_s\eta_s R_s^3\right.\\
&\left[B<(1+\frac{(e_3-e_1)}{e_1}I_{(ss)3}^2)^{1/2}(I_{(ss)k}I_{(ss)3}\delta e_{k1}+I_{(ss)k}I_{(ss)1}\delta e_{k3})>\right.\\
&-B<(1+\frac{(e_3-e_1)}{e_1}I_{(ss)3}^2)^{1/2}(\epsilon_{1rk}I_{(ss)k}I_{(ss)3}+\epsilon_{3rk}I_{(ss)k}I_{(ss)1})><\delta\omega_r>\\
&\left.+C<(1+\frac{(e_3-e_1)}{e_1}I_{(ss)3}^2)^{1/2}I_{(ss)1}I_{(ss)3}I_{(ss)k}I_{(ss)l}><\delta e_{kl}>\right]
\end{aligned}$$

$$
\begin{aligned}
&+2N_l\eta_l R_l^3 \Big[B < (1+\frac{(e_3-e_1)}{e_1}I^2_{(ll)3})^{1/2}(I_{(ll)k}I_{(ll)3}\delta e_{k1} + I_{(ll)k}I_{(ll)1}\delta e_{k3}) > \\
&-B < (1+\frac{(e_3-e_1)}{e_1}I^2_{(ll)3})^{1/2}(\epsilon_{1rk}I_{(ll)k}I_{(ll)3} + \epsilon_{3rk}I_{(ll)k}I_{(ll)1}) >< \delta\omega_r > \\
&+C < (1+\frac{(e_3-e_1)}{e_1}I^2_{(ll)3})^{1/2}I_{(ll)1}I_{(ll)3}I_{(ll)k}I_{(ll)l} >< \delta e_{kl} >\Big] \\
&+(R_sR_l)^{1/2}(R_l+R_s)(R_sN_s\eta_s + R_lN_l\eta_l) \\
&\Big[B < (1+\frac{(e_3-e_1)}{e_1}I^2_{(sl)3})^{1/2}(I_{(sl)k}I_{(sl)3}\delta e_{k1} + I_{(sl)k}I_{(sl)1}\delta e_{k3}) > \\
&-B\Big[< (1+\frac{(e_3-e_1)}{e_1}I^2_{(sl)3})^{1/2}(\epsilon_{1rk}I_{(sl)k}I_{(sl)3} \\
&+\epsilon_{3rk}I_{(sl)k}I_{(sl)1}) >< \delta\omega_r >\Big] \\
&+C < (1+\frac{(e_3-e_1)}{e_1}I^2_{(sl)3})^{1/2}I_{(sl)1}I_{(sl)3}I_{(sl)k}I_{(sl)l} >< \delta e_{kl} >\Big]
\end{aligned}
\tag{5.120}
$$

and then

$$
\begin{aligned}
C^*_{1313} &= \frac{(-e_1)^{1/2}}{4\pi VB(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\
&\Big\{2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2 + (R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2)\Big\} \\
&\left\{Bf_3\left(\frac{e_3}{e_1}\right) + C\left[\frac{-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(\frac{e_3}{e_1}-\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)}{\frac{e_3}{e_1}-1}\right]\right\} \\
&-B\Big\{2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2 + (R_sR_l)^{1/2}(R_l+R_s)(R_sN_s\eta_s + R_lN_l\eta_l)\Big\} \\
&\left(\frac{2f_2\left(\frac{e_3}{e_1}\right) - f_3\left(\frac{e_3}{e_1}\right)}{2f_2\left(\frac{e_3}{e_1}\right) - f_3\left(\frac{e_3}{e_1}\right)}\right).
\end{aligned}
\tag{5.121}
$$

Thus, we have the five independent effective elastic moduli, for an initial biaxial strain acting upon a binary packing of infinitely rough spheres.

Considering also the case of perfectly smooth spheres we see that the moduli now reduce to:

$$
\begin{aligned}
C^*_{1111} &= \frac{(-e_1)^{1/2}}{2\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))} \\
&\Big\{2R_s^3N_s^2\eta_s^2 + 2R_l^3N_l^2\eta_l^2(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2)\Big\} \\
&\left\{\frac{3}{8}\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2} + \left(\frac{1}{2}-\frac{e_3}{e_1}\right)f_2\left(\frac{e_3}{e_1}\right)}{\frac{e_3}{e_1}-1} + f_3\left(\frac{e_3}{e_1}\right)\right]\right\},
\end{aligned}
$$

$$C^*_{1122} = \frac{(-e_1)^{1/2}}{16\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}$$
$$\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\right\}$$
$$\left\{\frac{(\frac{1}{2}-\frac{e_3}{e_1})f_2\left(\frac{e_3}{e_1}\right)+\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}}{\frac{e_3}{e_1}-1}+f_3\left(\frac{e_3}{e_1}\right)\right\},$$

$$C^*_{1133} = \frac{(-e_1)^{1/2}}{4\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}$$
$$\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\right\}$$
$$\left\{\frac{(\frac{e_3}{e_1})-\frac{1}{2})f_2\left(\frac{e_3}{e_1}\right)-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}}{\frac{e_3}{e_1}-1}\right\},$$

$$C^*_{3333} = \frac{(-e_1)^{1/2}}{2\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}$$
$$\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\right\}$$
$$\left\{\left[\frac{\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+-\frac{1}{2}f_2\left(\frac{e_3}{e_1}\right)}{\frac{e_3}{e_1}-1}\right]\right\},$$

$$C^*_{1313} = \frac{(-e_1)^{1/2}}{4\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}$$
$$\left\{2R_s^3N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\right\}$$
$$\left\{\left[\frac{-\frac{1}{3}\left(\frac{e_3}{e_1}\right)^{3/2}+\left(\frac{e_3}{e_1}-\frac{1}{2}\right)f_2\left(\frac{e_3}{e_1}\right)}{\frac{e_3}{e_1}-1}\right]\right\}. \tag{5.122}$$

5.4 Comparison with Results of Numerical Simulation

In Chapter 3, we discussed the work of Jenkins *et al.* [43], their experimental, numerical simulation and theoretical results which gave the numerical values found for the effective elastic moduli of a random packing of spheres under prescribed conditions. Now, we wish to calculate the numerical values obtained from our new theoretical expressions for these effective moduli. The calculation of these expressions has been presented earlier in this chapter. For comparison with the values found by Jenkins *et al.* [43] we are only concerned with those values obtained after an initial hydrostatic strain.

The expressions we have found in this chapter cannot actually be compared directly with the values found by Jenkins from Walton's theory [86]. Jenkins' work only gave values to parameters for a random packing of EQUAL sized spheres (it was his experiments and simulations that involved different sized spheres). In the next section we discuss the work of Dr. Luc Oger [62] who kindly ran some simulations to help us determine these unknown values.

5.5 Calculation of the Co-ordination Number of Each Sphere

In their paper, Oger *et al.* [63] deal with the mechanical and electrical properties of particle packings by reducing the problem to that of a random packing of spheres, both equal sized and binary mixtures. We make use of their results as it is necessary to differentiate between the different types of grain-grain contact within a binary packing.

In a binary packing of spheres it is necessary to distinguish between the different types of contact. Hence, in a mixture of two different sphere sizes 1 and 2, in the relative proportions n_1 and n_2, Dodds [29] defines the different co-ordination numbers as follows:

- the mean co-ordination number C, which is defined to be the average number of contacts per sphere
- the mean co-ordination number c_i which is the average number of contacts for a particular sphere of type i
- the mean partial co-ordination number p_{ij}, this is the average number of contacts on spheres of type i by spheres of type j.

These co-ordination numbers are then related by the following equations:

$$\begin{aligned} C &= n_1 c_1 + n_2 c_2, \\ c_1 &= p_{11} + p_{12}, \\ c_2 &= p_{21} + p_{22}, \\ n_1 p_{12} &= n_2 p_{21}. \end{aligned} \tag{5.123}$$

Also introducing the relative fractions t_{ij} of different types of contacts between the spheres, in a binary mixture such as we are considering

$$t_{11} + t_{12} + t_{22} = 1,$$

$$\begin{aligned} t_{11} &= \frac{n_1 p_{11}}{C}, \\ t_{22} &= \frac{n_2 p_{22}}{C}, \\ t_{12} = t_{21} &= \frac{n_1 p_{12}}{C} = \frac{n_2 p_{21}}{C}. \end{aligned} \tag{5.124}$$

Oger *et al.* [63] made numerically simulated packings of binary mixtures of spheres with diameter ratios in the range 1 to 3.5 to find values for these quantities. These simulations were developed by Powell, whose work [64], [65], [66] and [67] describes the simulations in more detail. The packing was constructed one sphere at a time, positioning each in contact with a sphere already in the packing, chosen at random, and two other neighbouring spheres. Building this up layer by layer along the z-axis, periodic boundary conditions are imposed in the x- and y-directions. The porosity of a packing of two different sized spheres varies only slightly from 0.4 with the concentration of the small spheres. The mean total co-ordination number C is around 6.

In a real packing it can be hard to obtain an exact number for the co-ordination number as it may not be clear if two spheres are actually in contact or just very close. Some of the experimental techniques mentioned in chapter 1 experience this problem, they all use different techniques and can lead to very different answers. In their paper, Troadec and Dodds [82] describe the different kinds of 'contact' that may occur. These are classed according to the distance L between the centres of two equal sized spheres and can be separated into 4 classes:

- A real contact, $L = 2R$, where R is the radius of the spheres. This co-ordination number is around 6,
- A near contact, $2R < L < 2.1R$, yields a co-ordination number between 7 and 8.5,
- A close contact, $2R < L < 2.2R$, yields a co-ordination number between 7.7 and 9.3,
- A near neighbour, $L < 2\sqrt{2}R$, which gives a co-ordination number between 9 and 13.4. The Voronoi tessellation which gives this maximum value of 13.4 is a theoretical model discussed by Dodds [29] in which the space is paved with polygons representing the sphere positions and without any gaps.

Oger *et al.* [63] do consider these different type of contact, but here we are only concerned with the first class - real contacts. The maximum co-ordination number that can be attained in this situation is 12, it will only rise above this upon consideration of near neighbours.

A problem arises for sphere diameter-ratios greater than 6.46, in this case the small grains will start to fall through the gap formed by three large grains and segregation effects may become important. The packing would no longer be homogeneous. We will only consider sphere diameter-ratios less than this and so are not concerned with these effects.

To use these results for the comparison of our expressions derived in the previous section, with the results of Jenkins *et al.* [43], we require that the diameter ratio, $d_1/d_2 = 1.7$, with the proportion of small spheres, $n_1 = 0.91$ and the proportion of larger spheres $n_2 = 0.09$ (there were 392 spheres of radius 0.1075mm and 40 of radius 0.1825mm in the simulations discussed by Jenkins). However, to obtain a broader view on how the moduli change with different proportions of small to large spheres and different diameter-ratios, in the final section of this chapter we shall consider a range of different values for these.

Concentrating for now on obtaining comparable results to Jenkins, we note that in their paper, Oger *et al.* [63] only give some results for the diameter ratio $d_1/d_2 = 3$. Dr. Oger kindly sent the results of simulations to determine the values of the co-ordination numbers for $d_1/d_2 = 1.7$ as we require [62]. He found that in a packing of 16717 small spheres and 1383 large then the average co-ordination number of each sphere is $C = 6.00$, thus it is indeed 'close to 6' as mentioned in the discussion above. This percentage ratio, 92.4% of the packing consisting of small spheres, is not quite the same as that used in the numerical simulations discussed by Jenkins *et al.* [43], there 90.7% of the spheres were small. However, even though the simulations are not identical, the results will still enable us to get some idea of how the large spheres alter the values of the effective elastic moduli.

The other values found from Dr. Oger's simulations are given below, where the subscript l refers to large spheres and similarly, s to the small spheres, to make the notation more consistent with what has already been done:

$$c_l = 10.35936, \quad c_s = 5.64467,$$

$$p_{ll} = 1.49964, \quad p_{ss} = 4.91260, \quad p_{ls} = 8.85972, \quad p_{sl} = 0.73207,$$

$$t_{ll} = 0.01908, \quad t_{ss} = 0.75559, \quad t_{ls} = 0.22533.$$

For comparison with our notation we see that $c_l = \eta_l + \eta_{ls} = 10.35936$, $c_s = \eta_s + \eta_{sl} = 5.64467$, $p_{ll} = \eta_l = 1.49964$, $p_{ss} = \eta_s = 4.91260$, $p_{ls} = \eta_{ls} = 8.85972$ and $p_{sl} = \eta_{sl} = 0.73207$, which can all be substituted into the new expressions we have found for the effective moduli of the packing.

Thus, now recalling equations (5.91) and (5.90), we calculate the new values for the effective moduli. The expression for the effective shear modulus μ^*, is

$$\begin{aligned} \mu^* &= \frac{(-e)^{1/2}(5B+C)}{15\pi VB(2B+C)(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2N_s^2\eta_s^2R_s^3 \\ &\quad +2N_l^2\eta_l^2R_l^3+(R_sR_l)^{1/2}(R_s+R_l)(N_s^2\eta_{sl}^2R_s+N_l^2\eta_{ls}^2R_l)\} \end{aligned} \tag{5.125}$$

and that for the effective bulk modulus:

$$\begin{aligned} \kappa^* &= \frac{(-e)^{1/2}}{9\pi VB(N_s(\eta_s+\eta_{sl})+N_l(\eta_l+\eta_{ls}))}\{2R_s^2N_s^2\eta_s^2+2R_l^3N_l^2\eta_l^2 \\ &\quad +(R_sR_l)^{1/2}(R_s+R_l)(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)\}. \end{aligned} \tag{5.126}$$

Substituting in the values of each parameter, the first of these give us a value for the effective shear modulus of $\mu^* = 186$MPa. The previous theoretical value, found by Jenkins *et al.* [43] using Walton's theory, was 338MPa and so we have reduced the modulus by 45%. This new value is much closer to the 127MPa found by Jenkins *et al.* [43] in their numerical simulations.

We also find, from the second equation above, that the new value for the bulk modulus, κ^*, is 135MPa. Thus we again see a dramatic reduction in the value of the modulus predicted by the binary packing theory. In fact the new value is 55% of the previous theoretical value which was 245MPa, found from Walton [86]. Also, noticing that

Jenkins *et al.* [43], found a value of $\kappa^* = 185$MPa, we appear to have "overshot" the target. The table below shows a comparison of the values.

Modulus	Numerical Simulations	Walton's Theory	Theory (Different Sized Spheres)
Bulk	185MPa	245MPa	135MPa
Shear	127MPa	338MPa	186MPa

Both of these new predicted theoretical values clearly show that the affects of a small number of large spheres amongst a packing of small spheres can very significantly effect the theoretical properties of a packing. The new values then, are closer to those of Jenkins *et al.* [43], although the bulk modulus has decreased too much. In the next chapter, we will try to modify the results again. We shall again consider the influence of a perturbation of the uniform strain approximation upon these results. We would expect that the results found in this chapter using the uniform strain approximation for a binary packing would be significantly altered. We believe this to be the case due to the fact that the approximation becomes less accurate with decreasing co-ordination number. In this chapter we have been considering some co-ordination numbers as low as 0.7 for the number of large spheres in contact with a typical small one and 1.5 for the number of large spheres touching a typical large one. Thus, in the next chapter, we combine our two methods of calculation discussed in this chapter and chapter 3, in an attempt to make a further modification to the values of the predicted moduli.

5.5.1 Varying the Proportion of Spheres and Diameter Ratio

Before we continue with our attempts to modify the theory further, it is also interesting to briefly consider the effect the proportion of large spheres has upon the effective elastic moduli and also how these vary with the diameter ratio. Dr. Oger sent us some further results from his numerical simulations to enable us to do these calculations, these along with the new calculated value for the effective bulk and shear moduli are shown in the table below.

We have already concluded that for our particular parameters, a small number of large spheres amongst a packing of smaller spheres, significantly affects the values of the effective elastic moduli, when compared with those of a single size packing. The table on the following page clearly shows that this is true not just for the particular packing we have considered, but becomes more marked as we consider other proportions and diameter ratios.

As the proportion of large spheres increases, the effective moduli decrease in value. Hence, if we were able to consider an identical proportion of different sized spheres, that is a slightly greater proportion of large spheres, as considered by Jenkins *et al.* [43], then we would expect the moduli to decrease still further. This is good news for the shear modulus as we have dramatically reduced its value already and a further small reduction would bring the theoretical value even closer to that yielded by the numerical simulations. Unfortunately, this will also decrease the bulk modulus further which will not give the required result, its value has already decreased beyond the value found by the numerical simulations and so any further decrease will not improve the correlation between the two sets of results.

We can also note from the table that as the diameter ratio increases the effective moduli again decrease. Both of these conclusions show us that we must not discount the effect a size difference between spheres in a random packing has upon the properties of that packing.

% of small spheres	Diameter ratio	N_s	N_l	η_s	η_{sl}	η_l	$\eta_l s$	κ^* (MPa)	μ^* (MPa)
100	1			5.36	0	0	0	245	338
88.0294	1.4	9229	1255	4.604182	0.998050	1.151394	7.098008	121	168
93.9389	1.4	11562	746	5.211036	0.541429	0.500000	8.087132	173	239
98.7533	1.4	7763	98	5.705526	0.134999	0.061224	8.704082	242	334
84.5810	1.7	11920	2173	3.903775	1.374832	2.174873	7.346986	92	127
91.1965	1.7	15228	1470	4.590885	0.917126	1.171429	9.173470	121	166
98.3625	1.7	20484	341	5.632884	0.211384	0.123167	11.173020	224	308
74.6299	2.0	9528	3239	2.800378	1.988140	3.548626	5.698981	68	94
84.0441	2.0	14111	2679	3.603076	1.480831	2.754013	7.577828	74	102
92.5529	2.0	21662	1743	4.635445	0.833118	1.598394	10.117040	112	155
84.5239	3.0	8531	1562	3.032470	1.643184	4.008963	8.160691	63	87
90.09059	3.0	10326	1033	3.793047	1.217897	3.359148	10.376574	65	90
95.1375	3.0	15398	787	4.428627	0.864528	2.468869	14.069885	88	121

Chapter 6

A Perturbation of the Uniform Strain Approximation for a Binary Packing of Spheres

As has been previously mentioned, this chapter describes our attempt to modify the expressions for the effective moduli by considering a combination of the method used in chapter 3 with that of chapter 5. We expect the results to be significantly different from both of these chapters for reasons we discuss below.

We consider a dense, random, binary packing of spheres and apply a compressive force to the boundary. We use the uniform strain approximation for binary spheres as a first approximation to describe the displacement of the centre of each sphere and the rotation of the sphere about an axis through its centre and then perturb the approximation. Using the equations of equilibrium, we calculate approximations to first order for the perturbations. In addition to these, we apply an additional incremental deformation to the boundary and again, using a perturbation of the uniform strain approximation, calculate expressions for the effective elastic moduli of the packing.

Chapter 3 considers a perturbation of the uniform strain approximation, for a packing of equal sized spheres. We showed in chapter 5 that a few large spheres can dramatically effect the moduli, hence we would expect significant changes here. Chapter 5 used the uniform strain approximation as a starting point, but some of the co-ordination numbers were very small and we know that the approximation becomes poor for such cases. Hence the reason we would again expect the results of this chapter to significantly differ from those of Chapter 5. Hopefully by the end of the chapter we will have discovered some of the reasons why Jenkins *et al.* [43] calculated such different values for the effective moduli using numerical simulations than those obtained using the uniform strain approximation.

We proceed in precisely the same manner as we have done throughout this thesis. To recalculate the effective moduli, we first apply an initial deformation to the boundary of the packing and calculate the forces acting across the contact areas. From these, the average stress is found. We further apply an incremental deformation to the boundary and again calculate the forces and average incremental stress. Then, from the relationship between this stress and the average incremental strain, we calculate the effective elastic moduli for the packing.

6.1 The Initial Problem

We consider a large dense random packing, containing spheres of two sizes. The position vector of the centre of the nth small sphere is $\mathbf{X}_{(s)}^{(n)}$ and the position vector of the centre of a typical large sphere, n, is $\mathbf{X}_{(l)}^{(n)}$. The displacement on the boundary, $\mathbf{u}$ is consistent with a uniform strain and hence

$$u_i = e_{ij}x_j. \tag{6.1}$$

The previous chapter dealt with the assumption that the centres of the spheres are displaced consistently with this uniform applied field, $u_{(s)i}^{(n)} = e_{ij}X_{(s)j}^{(n)}$ and $u_{(l)i}^{(n)} = e_{ij}X_{(l)j}^{(n)}$ and that the rotation terms satisfy $\omega_{(s)i}^{(n)} = \omega_{(s)i}^{(n')} = \Omega_{(s)i}$ and $\omega_{(l)i}^{(n)} = \omega_{(l)i}^{(n')} = \Omega_{(l)i}$. We wish to consider perturbations of this uniform strain approximation, $\tilde{u}_{(s)i}^{(n)}$ and $\tilde{\omega}_{(s)i}^{(n)}$, for each small sphere and $\tilde{u}_{(l)i}^{(n)}$ and $\tilde{\omega}_{(l)i}^{(n)}$, for each large sphere. Thus, for a small sphere, the nth say, after the initial deformation the centre of this sphere has been displaced by an amount:

$$u_{(s)i}^{(n)} = e_{ij}X_{(s)j}^{(n)} + \tilde{u}_{(s)i}^{(n)} \tag{6.2}$$

and

$$\omega_{(s)i}^{(n)} = \Omega_{(s)i} + \tilde{\omega}_{(s)i}^{(n)} \tag{6.3}$$

and for the nth typical large sphere

$$u_{(l)i}^{(n)} = e_{ij}X_{(l)j}^{(n)} + \tilde{u}_{(l)i}^{(n)} \tag{6.4}$$

and

$$\omega_{(l)i}^{(n)} = \Omega_{(l)i} + \tilde{\omega}_{(l)i}^{(n)}. \tag{6.5}$$

Initially, we again restrict our attention to a packing of infinitely rough spheres.

We have already seen in Chapter 5, that the general expression for the force acting on the nth small sphere, due to its contact with another small sphere, n', is

$$\begin{aligned} F_{(ss)i}^{(nn')} &= \frac{(2R_s)^{1/2}}{3\pi B(2B+C)} \left\{2B[(u_{(s)p}^{(n')} - u_{(s)p}^{(n)})I_{(ss)p}^{(nn')}]^{1/2}(u_{(s)i}^{(n')} - u_{(s)i}^{(n)} \right. \\ & \left. + R_s\epsilon_{ijk}(\omega_{(s)j}^{(n')} + \omega_{(s)j}^{(n)})I_{(ss)k}^{(nn')}) + C[(u_{(s)p}^{(n')} - u_{(s)p}^{(n)})I_{(ss)p}^{(nn')}]^{3/2}I_{(ss)i}^{(nn')}\right\}, \end{aligned} \tag{6.6}$$

where B and C are the constants determined previously in terms of the Lamé moduli. Similarly, the force acting on a large sphere, n, due to its contact with another large one, n', is

$$\begin{aligned} F_{(ll)i}^{(nn')} &= \frac{(2R_l)^{1/2}}{3\pi B(2B+C)} \left\{2B[(u_{(l)p}^{(n')} - u_{(l)p}^{(n)})I_{(ll)p}^{(nn')}]^{1/2}(u_{(l)i}^{(n')} - u_{(l)i}^{(n)} \right. \\ & \left. + R_l\epsilon_{ijk}(\omega_{(l)j}^{(n')} + \omega_{(l)j}^{(n)})I_{(ll)k}^{(nn')}) + C[(u_{(l)p}^{(n')} - u_{(l)p}^{(n)})I_{(ll)p}^{(nn')}]^{3/2}I_{(ll)i}^{(nn')}\right\} \end{aligned} \tag{6.7}$$

and the force acting on a small sphere, n, due to its contact with a large sphere n' is

$$\begin{aligned} F_{(sl)i}^{(nn')} &= \frac{2(R')^{1/2}}{3\pi B(2B+C)} \left\{2B[(u_{(l)p}^{(n')} - u_{(s)p}^{(n)})I_{(sl)p}^{(nn')}]^{1/2}(u_{(l)i}^{(n')} - u_{(s)i}^{(n)} \right. \\ & \left. + \epsilon_{ijk}(R_l\omega_{(l)j}^{(n')} + R_s\omega_{(s)j}^{(n)})I_{(sl)k}^{(nn')}) + C[(u_{(l)p}^{(n')} - u_{(s)p}^{(n)})I_{(sl)p}^{(nn')}]^{3/2}I_{(sl)i}^{(nn')}\right\}. \end{aligned} \tag{6.8}$$

In order to calculate approximations for the perturbation terms we consider equilibrium of these forces and their moments.

In order to calculate the forces following, in particular, an initial hydrostatic strain, we must expand terms such as

$$[(u_{(l)p}^{(n')} - u_{(s)p}^{(n)})I_{(sl)p}^{(nn')}]^{1/2} = (R_s + R_l)^{1/2}(-e)^{1/2}\left[1 - \frac{1}{2(R_s+R_l)e}(\tilde{u}_{(l)p}^{(n')} - \tilde{u}_{(s)p}^{(n)})I_{(sl)p}\right.$$

$$-\frac{1}{8(R_s+R_l)^2e^2}(\tilde{u}^{(n')}_{(l)p}-\tilde{u}^{(n)}_{(s)p})(\tilde{u}^{(n')}_{(l)q}-\tilde{u}^{(n)}_{(s)q})I_{(sl)p}I_{(sl)q}\Big] \tag{6.9}$$

and

$$\begin{aligned}[(u^{(n')}_{(l)p}-u^{(n)}_{(s)p})I^{(nn')}_{(sl)p}]^{3/2} &= (R_s+R_l)^{3/2}(-e)^{3/2}\Big[1-\frac{3}{2(R_s+R_l)e}(\tilde{u}^{(n')}_{(l)p}-\tilde{u}^{(n)}_{(s)p})I_{(sl)p} \\ &+\frac{3}{8(R_s+R_l)^2e^2}(\tilde{u}^{(n')}_{(l)p}-\tilde{u}^{(n)}_{(s)p})(\tilde{u}^{(n')}_{(l)q}-\tilde{u}^{(n)}_{(s)q})I_{(sl)p}I_{(sl)q}\Big],\end{aligned} \tag{6.10}$$

which both occur in the expression for $\mathbf{F}^{(nn')}_{(sl)}$. Very similar expansions occur in the expressions for $\mathbf{F}^{(nn')}_{(ss)}$ and $\mathbf{F}^{(nn')}_{(ll)}$.

Now, in particular for the nth small sphere, we require equilibrium of the forces and moments acting, due to its contact with other spheres:

$$\sum_{n'\ small}\mathbf{F}^{(nn')}_{(ss)}+\sum_{n'\ large}\mathbf{F}^{(nn')}_{(sl)}=\mathbf{0} \tag{6.11}$$

and

$$\sum_{n'\ small}\mathbf{F}^{(nn')}_{(ss)}\wedge\mathbf{I}^{(nn')}_{(ss)}+\sum_{n'\ large}\mathbf{F}^{(nn')}_{(sl)}\wedge\mathbf{I}^{(nn')}_{(sl)}=\mathbf{0}, \tag{6.12}$$

where $\mathbf{F}^{(nn')}_{(ss)i}$ and $\mathbf{F}^{(nn')}_{(sl)i}$ are as given previously. Similarly, for equilibrium of a large sphere, we require

$$\sum_{n'\ large}\mathbf{F}^{(nn')}_{(ll)}+\sum_{n'\ small}\mathbf{F}^{(nn')}_{(ls)}=\mathbf{0} \tag{6.13}$$

and

$$\sum_{n'\ large}\mathbf{F}^{(nn')}_{(ll)}\wedge\mathbf{I}^{(nn')}_{(ll)}+\sum_{n'\ large}\mathbf{F}^{(nn')}_{(ls)}\wedge\mathbf{I}^{(nn')}_{(ls)}=\mathbf{0}. \tag{6.14}$$

Following the same method used in chapter 3, we substitute the general force expressions for a binary packing, into the first pair of these equilibrium conditions, equations (6.11) and (6.12). As in Chapter 3, we again have to make some assumptions about the order of terms, in order to try and reduce the equations of equilibrium to first order. This then allows us to find first order approximations for $\tilde{u}^{(n)}_{(s)i}$ and $\tilde{\omega}^{(n)}_{(s)i}$.

We restrict ourselves to consider an initial hydrostatic strain, this is the initial compression we require for comparison of our results with Jenkins *et al.* [43]. Thus, we have $e_{ij} = e\delta_{ij}$ and also $\Omega_{(l)i} = \Omega_{(s)i} = 0$ and find that the first order approximation for $\tilde{u}^{(n)}_{(s)i}$ is given by:

$$\tilde{u}^{(n)}_{(s)i} = -\frac{6Ae(2R_s^2\eta_s J^{(n)}_{(ss)i} + (R_lR_s)^{1/2}(R_l + R_s)\eta_{sl}J^{(n)}_{(sl)i})}{(R_s\eta_s + (R_lR_s)^{1/2}\eta_{sl})}. \tag{6.15}$$

The definitions of $J^{(n)}_{(ss)i}$ and $J^{(n)}_{(sl)i}$ are very similar to that of $J^{(n)}_i$, which in chapter 3 was defined as:

$$J^{(n)}_i = \frac{1}{\eta^{(n)}}\sum_{n'} I^{(nn')}_i.$$

We now define

$$J^{(n)}_{(ss)i} = \frac{1}{\eta^{(n)}_s}\sum_{n'\ small} I^{(nn')}_{(ss)i} \tag{6.16}$$

and

$$J^{(n)}_{(sl)i} = \frac{1}{\eta^{(n)}_{sl}}\sum_{n'\ large} I^{(nn')}_{(sl)i}. \tag{6.17}$$

All other quantities are as previously defined in other chapters, but as a reminder we have R_l and R_s are the radii of large and small spheres, respectively and

$$A = \frac{2B + C}{14B + 3C},$$

where B and C are constants defined in terms of the Lamé constants for the medium. Each η corresponds to a co-ordination number.

From the condition that ensures equilibrium of moments, we also find a first order approximation for $\tilde{\omega}^{(n)}_{(s)i}$, this is

$$\tilde{\omega}^{(n)}_{(s)i} = 0. \tag{6.18}$$

Thus now, we approximate the displacement of the centre of the nth small sphere as follows:

$$u^{(n)}_{(s)i} = e_{ij}X^{(n)}_{(s)j} - \frac{6Ae(2R_s^2\eta_s J^{(n)}_{(ss)i} + (R_lR_s)^{1/2}(R_l + R_s)\eta_{sl}J^{(n)}_{(sl)i})}{(R_s\eta_s + (R_lR_s)^{1/2}\eta_{sl})} \tag{6.19}$$

and the rotation about an axis through its centre as

$$\omega^{(n)}_{(s)i} = 0. \tag{6.20}$$

Similarly, the displacement of the centre of the nth large sphere is found by considering the equilibrium of a typical large sphere and we have

$$u_{(l)i}^{(n)} = e_{ij}X_{(l)j}^{(n)} - \frac{6Ae(2R_l^2\eta_l J_{(ll)i}^{(n)} + (R_lR_s)^{1/2}(R_l+R_s)\eta_{ls}J_{(ls)i}^{(n)})}{(R_l\eta_l + (R_lR_s)^{1/2}\eta_{ls})} \tag{6.21}$$

and

$$\omega_{(l)i}^{(n)} = 0. \tag{6.22}$$

We define $J_{(ll)i}^{(n)}$ and $J_{(ls)i}^{(n)}$ in the obvious way:

$$J_{(ll)i}^{(n)} = \frac{1}{\eta_l^{(n)}} \sum_{n'\ large} I_{(ll)i}^{(nn')} \tag{6.23}$$

and

$$J_{(ls)i}^{(n)} = \frac{1}{\eta_{ls}^{(n)}} \sum_{n'\ small} I_{(ls)i}^{(nn')}. \tag{6.24}$$

Using these expressions for the displacements and rotations, we can find the force acting on the nth sphere due to its contact with the n'th. Substituting these into the general force equations (6.6), (6.7) and (6.8), we calculate very lengthy expressions for all the forces, $\mathbf{F}_{(ss)}^{(nn')}$, $\mathbf{F}_{(ll)}^{(nn')}$, $\mathbf{F}_{(sl)}^{(nn')} = -\mathbf{F}_{(ls)}^{(n'n)}$, acting across the contact areas within the packing.

As the expressions for these forces are so lengthy, only one will be included here, $\mathbf{F}_{(sl)i}^{(nn')}$. In its entirety, this would still be too long for inclusion and so we leave the expression containing general displacement expressions such as $\tilde{u}_{(s)i}^{(n)}$ and into which we substitute the approximation found above. We have

$$\begin{aligned} F_{(sl)i}^{(nn')} = & \frac{(R_sR_l)^{1/2}(-e)^{1/2}}{3\pi B(2B+C)} \Big\{ 2B\Big[-(R_s+R_l)eI_{(sl)i} + \tilde{u}_{(l)i}^{(n')} - \tilde{u}_{(s)i}^{(n)} \\ & + \frac{1}{2}(\tilde{u}_{(l)p}^{(n')} - \tilde{u}_{(s)p}^{(n)})I_{(sl)p}I_{(sl)i} \\ & - \frac{1}{2(R_s+R_l)e}(\tilde{u}_{(l)i}^{(n')} - \tilde{u}_{(s)i}^{(n)})(\tilde{u}_{(l)p}^{(n')} - \tilde{u}_{(s)p}^{(n)})I_{(sl)p} \\ & + \frac{1}{8(R_s+R_l)e}(\tilde{u}_{(l)p}^{(n')} - \tilde{u}_{(s)p}^{(n)})(\tilde{u}_{(l)q}^{(n')} - \tilde{u}_{(s)q}^{(n)})I_{(sl)p}I_{(sl)q}I_{(sl)i}\Big] \\ & + C\Big[-e(R_s+R_l)I_{(sl)i} + \frac{3}{2}(\tilde{u}_{(l)p}^{(n')} - \tilde{u}_{(s)p}^{(n)})I_{(sl)p}I_{(sl)i} \\ & - \frac{3}{8(R_s+R_l)e}(\tilde{u}_{(l)p}^{(n')} - \tilde{u}_{(s)p}^{(n)})(\tilde{u}_{(l)q}^{(n')} - \tilde{u}_{(s)q}^{(n)})I_{(sl)p}I_{(sl)q}I_{(sl)i}\Big]\Big\}. \end{aligned} \tag{6.25}$$

The Average Stress

Having found the forces acting across each contact area, the next stage in the problem is to calculate the average stress throughout the medium. From equation (5.46), we have the following general expression for this stress

$$\begin{aligned} < \sigma_{ij} > \;=\; & -\frac{1}{2V}\{N_s\eta_s R_s(< I^{(nn')}_{(ss)i}F^{(nn')}_{(ss)j} > + < I^{(nn')}_{(ss)j}F^{(nn')}_{(ss)i} >) \\ & +N_l\eta_l R_l(< I^{(nn')}_{(ll)i}F^{(nn')}_{(ll)j} > + < I^{(nn')}_{(ll)j}F^{(nn')}_{(ll)i} >) \\ & +N_s\eta_{sl} R_s(< I^{(nn')}_{(sl)i}F^{(nn')}_{(sl)j} > + < I^{(nn')}_{(sl)j}F^{(nn')}_{(sl)i} >) \\ & +N_l\eta_{ls} R_l(< I^{(nn')}_{(ls)i}F^{(nn')}_{(ls)j} > + < I^{(nn')}_{(ls)j}F^{(nn')}_{(ls)i} >)\}. \end{aligned} \quad (6.26)$$

Substituting in the lengthy force expressions just calculated, the resulting stress involves statistical parameters of the packing. These are similar to α_{ij}, defined in equation (3.30), although we have several this time. Assuming that they are isotropic as before, we define

$$\begin{aligned} \alpha_{(ss)ij} &= < I^{(nn')}_{(ss)i}J^{(n)}_{(ss)j} >= \alpha_{ss}\delta_{ij} \\ \alpha_{(ll)ij} &= < I^{(nn')}_{(ll)i}J^{(n)}_{(ll)j} >= \alpha_{ll}\delta_{ij} \\ \alpha_{(sl)ij} &= < I^{(nn')}_{(sl)i}J^{(n)}_{(sl)j} >= \alpha_{sl}\delta_{ij} \\ \alpha_{(ls)ij} &= < I^{(nn')}_{(ls)i}J^{(n)}_{(ls)j} >= \alpha_{ls}\delta_{ij} \end{aligned} \quad (6.27)$$

where the average value $< . >$ is calculated over all contacts. Thus, calculation of each α, reduces to a sum of $J^{(n)}_i$ squared terms, for example, if $N(s,l)\eta(s,l)$ is the total number of contacts, $N(s,l)\eta(s,l) = N_s(\eta_s + \eta_{sl}) + N_l(\eta_l + \eta_{ls})$, then

$$\alpha_{ss} = \frac{\eta^{(n)}_{(s)}}{3N(s,l)\eta(s,l)}\sum_n J_{(ss)i}J_{(ss)i}, \quad (6.28)$$

summing over n, that is all spheres. Each of the αs above can be written in this way. The summation over which each is taken reduces, since the various $J^{(n)}_i$s will not exist for all types of sphere contact. For example, α_{ss} reduces to

$$\alpha_{ss} = \frac{\eta^{(n)}_{(s)}}{3N(s,l)\eta(s,l)}\sum_{n\ small} J_{(ss)i}J_{(ss)i}.$$

We have cross terms which also arise and these cannot be defined in quite the same way. A term which we define as α_{sssl} can in fact arise from two different terms. These are $< I^{(nn')}_{(ss)i} J^{(n)}_{(sl)j} >$ and $< I^{(nn')}_{(sl)i} J^{(n)}_{(ss)j} >$, but multiplied by different combinations of the co-ordination numbers. To allow for this and so that we do not have to use two separate parameters for each of these terms we define

$$\begin{aligned}
\alpha_{(sssl)ij} &= \frac{1}{3N(s,l)\eta(s,l)} \sum_n J^{(n)}_{(ss)i} J^{(n)}_{(sl)i} = \alpha_{sssl}\delta_{ij} \\
\alpha_{(llls)ij} &= \frac{1}{3N(s,l)\eta(s,l)} \sum_n J^{(n)}_{(ll)i} J^{(n)}_{(ls)i} = \alpha_{llls}\delta_{ij}
\end{aligned} \tag{6.29}$$

The variations in multiples of co-ordination number are then included in the general theoretical expression at each stage, rather than in the numerical calculation on the computer. Hence, for example, we have

$$< I^{(nn')}_{(ss)i} J^{(n)}_{(sl)j} >= \eta_s \alpha_{sssl} \delta_{ij} \tag{6.30}$$

whereas

$$< I^{(nn')}_{(sl)i} J^{(n)}_{(ss)j} >= \eta_{sl} \alpha_{sssl} \delta_{ij}. \tag{6.31}$$

We calculate average values for each α by using computer simulation. The programs are similar to those used to determine α in Chapter 3 and will be discussed later in this chapter.

As in chapter 3 it is not just terms such as $\langle I^{(nn')}_{(ss)i} J^{(n)}_{(ss)j} \rangle$ which arise in these calculations, but also more complicated averages, for example, $\langle I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} I^{(nn')}_{(ss)k} J^{(n)}_{(ss)l} \rangle$, $\langle I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} J^{(n)}_{(ss)k} J^{(n)}_{(ss)l} \rangle$ and $\langle I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} J^{(n)}_{(sl)k} J^{(n)}_{(sl)l} \rangle$. However, all the terms that occur at this stage of the problem can in fact be reduced to expressions in terms of the known αs. In Chapter 3, we found expressions for similar terms to these three using the properties of isotropic tensors. For example, assuming $\langle I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} I^{(nn')}_{(ss)k} J^{(n)}_{(ss)l} \rangle$, is a fourth order, isotropic tensor then it can be written as a linear combination of $\delta_{ij}\delta_{kl}$, $\delta_{ik}\delta_{jl}$ and $\delta_{il}\delta_{jk}$. It must be symmetric upon interchange of any two of i, j, k and the only combination that satisfies this is:

$$< I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} I^{(nn')}_{(ss)k} J^{(n)}_{(ss)l} >= C_1(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

where C_1 is a constant. As in Chapter 3, since $I^{(nn')}_{(ss)p} I^{(nn')}_{(ss)p} = 1$ then setting $i = j$ gives $C_1 = \frac{\alpha_{ss}}{5}$.

Determining the other expressions in a similar way then, in particular, the three averages mentioned become

$$< I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} I^{(nn')}_{(ss)k} J^{(n)}_{(ss)l} >= \frac{\alpha_{ss}}{5}(\delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}),$$

$$< I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} J^{(n)}_{(ss)k} J^{(n)}_{(ss)l} >= \frac{\alpha_{ss}}{3}\delta_{ij}\delta_{kl}$$

and

$$< I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} J^{(n)}_{(sl)k} J^{(n)}_{(sl)l} >= \frac{\eta_s \alpha_{sl}}{3\eta_{sl}}\delta_{ij}\delta_{kl}.$$

Some further manipulations with these averages and parameters must be done in order to calculate the average stress as we wish to do. It is not immediately obvious from the definitions of the αs how a term such as $< I^{(nn')}_{(ls)i} J^{(n')}_{(ss)j} >$ can be written down. However, with some rearranging and using the fact that

$$I^{(nn')}_{(ls)i} = -I^{(n'n)}_{(sl)i},$$

we find the following is true:

$$< I^{(nn')}_{(ls)i} J^{(n')}_{(ss)j} >= -\eta_{sl}\alpha_{sssl}. \tag{6.32}$$

Now, putting all of these manipulations together, the expression for the average stress is thus given in terms of the α parameters as:

$$\begin{aligned}
< \sigma_{ij} > \; = \\
& -\frac{2(-e)^{3/2}}{3\pi V B}\Bigg\{ R_s^2 N_s \eta_s \Bigg[\frac{2R_s N_s \eta_s}{3N} - 18A\frac{(2R_s^2\eta_s\alpha_{ss} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\eta_s\alpha_{sssl})}{(R_s\eta_s + (R_sR_l)^{1/2}\eta_{sl}^2)} \\
& \quad + \frac{9A^2}{2R_s}\frac{(4R_s^4\eta_s^2\alpha_{ss} + 4R_s^2\eta_s^2\eta_{sl}\alpha_{sssl} + (R_sR_l)(R_s+R_l)^2\eta_{sl}\eta_s\alpha_{sl})}{(R_s\eta_s + (R_sR_l)^{1/2}\eta_{sl})^2}\Bigg] \\
& \quad + R_l^2 N_l \eta_l \Bigg[\frac{2R_l N_l \eta_l}{3N} - 18A\frac{(2R_l^2\eta_l\alpha_{ll} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\eta_l\alpha_{llls})}{(R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls})^2} \\
& \quad + \frac{9A^2}{2R_l}\frac{(4R_l^4\eta_l^2\alpha_{ll} + 4R_l^2\eta_l^2\eta_{ls}\alpha_{llls} + (R_sR_l)(R_s+R_l)^2\eta_{ls}\eta_l\alpha_{ls})}{(R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls})^2}\Bigg] \\
& + (R_sR_l)^{1/2}(R_sN_s\eta_{sl} + R_lN_l\eta_{ls})\Bigg[\frac{(R_s+R_l)N_l n_{ls}}{3N} \\
& -9A\left(\frac{2R_s^2\eta_s\alpha_{ss} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl}}{(R_s\eta_s + (R_sR_l)^{1/2}\eta_{sl})} + \frac{2R_l^2\eta_l\alpha_{ll} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{ls}}{(R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls})}\right)
\end{aligned}$$

$$+\frac{9A^2}{2(R_s+R_l)}\left(\frac{4R_s^2\eta_s\eta_{sl}\alpha_{ss}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}^2\alpha_{sssl}+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}}{(R_s\eta_s+(R_sR_l)^{1/2}\eta_{sl})^2}\right.$$
$$\left.\left.\left.+\frac{4R_l^2\eta_l\eta_{ls}\alpha_{ll}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}^2\alpha_{llls}+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}}{(R_l\eta_l+(R_sR_l)^{1/2}\eta_{ls})^2}\right)\right]\right\}. \tag{6.33}$$

This is the expression we require.

These results have all been calculated for the case of infinitely rough spheres but as has been seen already in previous chapters, the calculations can also be done for a packing of perfectly smooth spheres. In this case, the force expressions are not nearly so lengthy and the equivalent expression to equation (6.25) is

$$\begin{aligned} F^{(nn')}_{(sl)i} &= \frac{(R_sR_l)^{1/2}(-e)^{1/2}}{3\pi B}\left\{-e(R_s+R_l)I_{(sl)i}+\frac{3}{2}(\tilde{u}^{(n')}_{(l)p}-\tilde{u}^{(n)}_{(s)p})I_{(sl)p}I_{(sl)i}\right. \\ &\left. -\frac{3}{8(R_s+R_l)e}(\tilde{u}^{(n')}_{(l)p}-\tilde{u}^{(n)}_{(s)p})(\tilde{u}^{(n')}_{(l)q}-\tilde{u}^{(n)}_{(s)q})I_{(sl)p}I_{(sl)q}I_{(sl)i}\right\}, \end{aligned} \tag{6.34}$$

with similar expressions also holding for $F^{(nn')}_{(ss)i}$ and $F^{(nn')}_{(ll)i}$. The average stress is now

$$\begin{aligned} <\sigma_{ij}> &= \\ & -\frac{2(-e)^{3/2}}{3\pi VB}\left\{R_s^2N_s\eta_s\left[\frac{2R_sN_s\eta_s}{3N}-6\frac{(2R_s^2\eta_s\alpha_{ss}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\eta_s\alpha_{sssl})}{(R_s\eta_s+(R_sR_l)^{1/2}\eta_{sl}^2)}\right.\right. \\ &\left. +\frac{1}{2R_s}\frac{(4R_s^4\eta_s^2\alpha_{ss}+4R_s^2\eta_s^2\eta_{sl}\alpha_{sssl}+(R_sR_l)(R_s+R_l)^2\eta_{sl}\eta_s\alpha_{sl})}{(R_s\eta_s+(R_sR_l)^{1/2}\eta_{sl})^2}\right] \\ & +R_l^2N_l\eta_l\left[\frac{2R_lN_l\eta_l}{3N}-6\frac{(2R_l^2\eta_l\alpha_{ll}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\eta_l\alpha_{llls})}{(R_l\eta_l+(R_sR_l)^{1/2}\eta_{ls})^2}\right. \\ &\left. +\frac{1}{2R_l}\frac{(4R_l^4\eta_l^2\alpha_{ll}+4R_l^2\eta_l^2\eta_{ls}\alpha_{llls}+(R_sR_l)(R_s+R_l)^2\eta_{ls}\eta_l\alpha_{ls})}{(R_l\eta_l+(R_sR_l)^{1/2}\eta_{ls})^2}\right] \\ & +(R_sR_l)^{1/2}(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})\left[\frac{(R_s+R_l)N_ln_{ls}}{3N}\right. \\ & -3\left(\frac{2R_s^2\eta_s\alpha_{ss}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl}}{(R_s\eta_s+(R_sR_l)^{1/2}\eta_{sl})}+\frac{2R_l^2\eta_l\alpha_{ll}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{ls}}{(R_l\eta_l+(R_sR_l)^{1/2}\eta_{ls})}\right) \\ & +\frac{1}{2(R_s+R_l)}\left(\frac{4R_s^2\eta_s\eta_{sl}\alpha_{ss}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}^2\alpha_{sssl}+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}}{(R_s\eta_s+(R_sR_l)^{1/2}\eta_{sl})^2}\right. \\ &\left.\left.\left. +\frac{4R_l^2\eta_l\eta_{ls}\alpha_{ll}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}^2\alpha_{llls}+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}}{(R_l\eta_l+(R_sR_l)^{1/2}\eta_{ls})^2}\right)\right]\right\}. \end{aligned} \tag{6.35}$$

6.2 Calculation of the Effective Moduli

As with all our previous work to calculate the effective moduli, we impose an incremental deformation upon the initial configuration. A small sphere on the boundary will undergo a further displacement

$$\delta u_{(s)i} = \delta e_{ij} x_{(s)j} \tag{6.36}$$

and similarly a large sphere will undergo a further displacement

$$\delta u_{(l)i} = \delta e_{ij} x_{(l)j}. \tag{6.37}$$

The uniform strain approximation, as used in Chapter 5, assumes that the centre of the nth small sphere would be displaced by an amount

$$\delta u^{(n)}_{(s)i} = \delta e_{ij} X^{(n)}_{(s)j} \tag{6.38}$$

and a similar expression holds for a large sphere. Again, perturbing this approximation as we have already done for the initial problem, then upon application of the boundary displacement, the centre of a typical small sphere, the nth say, is displaced by an amount

$$\delta u^{(n)}_{(s)i} = \delta e_{ij} X^{(n)}_{(s)j} + \delta \tilde{u}^{(n)}_{(s)i} \tag{6.39}$$

and rotates about an axis through its centre by an amount

$$\delta \omega_{(s)i} = \delta \Omega_{(s)i} + \delta \tilde{\omega}^{(n)}_{(s)i}. \tag{6.40}$$

A typical large sphere, the nth, is displaced by

$$\delta u^{(n)}_{(l)i} = \delta e_{ij} X^{(n)}_{(l)j} + \delta \tilde{u}^{(n)}_{(l)i} \tag{6.41}$$

and rotates by

$$\delta \omega_{(l)i} = \delta \Omega_{(l)i} + \delta \tilde{\omega}^{(n)}_{(l)i}. \tag{6.42}$$

Again, we consider the equilibrium of forces and moments acting on each sphere. These conditions allow us to find approximations for the perturbation terms. For a small sphere the following equations must hold, we have

$$\sum_{n'\ small} \delta\mathbf{F}^{(nn')}_{(ss)} + \sum_{n'\ large} \delta\mathbf{F}^{(nn')}_{(sl)} = \mathbf{0} \tag{6.43}$$

and

$$\sum_{n'\ small} \delta\mathbf{F}^{(nn')}_{(ss)} \wedge \mathbf{I}^{(nn')}_{(ss)} + \sum_{n'\ large} \delta\mathbf{F}^{(nn')}_{(sl)} \wedge \mathbf{I}^{(nn')}_{(sl)} = \mathbf{0} \tag{6.44}$$

and for a large sphere we have

$$\sum_{n'\ large} \delta\mathbf{F}^{(nn')}_{(ll)} + \sum_{n'\ small} \delta\mathbf{F}^{(nn')}_{(ls)} = \mathbf{0} \tag{6.45}$$

and

$$\sum_{n'\ large} \delta\mathbf{F}^{(nn')}_{(ll)} \wedge \mathbf{I}^{(nn')}_{(ll)} + \sum_{n'\ small} \delta\mathbf{F}^{(nn')}_{(sl)} \wedge \mathbf{I}^{(nn')}_{(sl)} = \mathbf{0}. \tag{6.46}$$

The incremental forces acting on the nth sphere due to its contact with the n'th sphere, that is $\delta\mathbf{F}^{(nn')}_{(ss)}$, $\delta\mathbf{F}^{(nn')}_{(sl)} = -\delta\mathbf{F}^{(n'n)}_{(ls)}$ and $\delta\mathbf{F}^{(nn')}_{(ll)}$, are given in equations (5.71), (5.73) and (5.72), respectively. We expand the terms in these expressions, as we did for the initial part of the problem, equations (6.6), (6.7) and (6.8) and then substitute these expressions into the equilibrium equations above. We again make assumptions about the order of the terms in order to enable us to calculate first order approximations for $\delta\tilde{u}_i^{(n)}$ and $\delta\tilde{\omega}_i^{(n)}$. We find that to first order, the centre of the nth small sphere is displaced by an amount

$$\begin{aligned}
\delta u^{(n)}_{(s)i} &= \delta e_{ij} X^{(n)}_{(s)i} \\
&- \frac{3}{(6B+C)} \left\{ 2B(1-A)\delta e_{ik} \frac{(2R_s^2\eta_s J^{(n)}_{(ss)k} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl} J^{(n)}_{(sl)k})}{R_s\eta_s + (R_sR_l)^{1/2}\eta_{sl}} \right. \\
&\qquad + C\delta e_{rt} \left(\frac{2R_s^2\eta_s N^{(n)}_{(ss)tri} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl} N^{(n)}_{(sl)tri}}{R_s\eta_s + (R_sR_l)^{1/2}\eta_{sl}} \right. \\
&\left.\left. - \frac{A}{5}(\delta_{tp}\delta_{ir} + \delta_{tr}\delta_{ip} + \delta_{it}\delta_{pr}) \left(\frac{2R_s^2\eta_s J^{(n)}_{(ss)p} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl} J^{(n)}_{(sl)p}}{R_s\eta_s + (R_sR_l)^{1/2}\eta_{sl}} \right) \right) \right\}
\end{aligned} \tag{6.47}$$

where $N^{(n)}_{(ss)tri}$ and $N^{(n)}_{(sl)tri}$ are defined in an analogous way to $N^{(n)}_{tri}$, which was seen previously in Chapter 3. However, the extra subscripts allow us to distinguish which size of spheres are used in the calculation. Thus we have

$$N^{(n)}_{(ss)tri} = \frac{1}{\eta_s} \sum_{n'\ small} I^{(nn')}_{(ss)t} I^{(nn')}_{(ss)r} I^{(nn')}_{(ss)i} \tag{6.48}$$

and

$$N^{(n)}_{(sl)tri} = \frac{1}{\eta_{sl}} \sum_{n'\ small} I^{(nn')}_{(sl)t} I^{(nn')}_{(sl)r} I^{(nn')}_{(sl)i}. \tag{6.49}$$

In this chapter we are purely interested in hydrostatic initial conditions and from the equation for equilibrium of moments we then also find that to first order:

$$\delta\omega^{(n)}_{(s)i} = 0. \tag{6.50}$$

The displacement of the centre of the nth large sphere is found in the same way by considering equilibrium of the nth large sphere, we calculate:

$$\begin{aligned} \delta u^{(n)}_{(l)i} &= \delta e_{ij} X^{(n)}_{(l)i} \qquad (6.51)\\ &-\frac{3}{(6B+C)}\Bigg\{2B(1-A)\delta e_{ik}\frac{(2R_l^2\eta_s J^{(n)}_{(ll)k} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}J^{(n)}_{(ls)k})}{R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls}} \\ &\qquad +C\delta e_{rt}\left(\frac{2R_l^2\eta_l N^{(n)}_{(ll)tri} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}N^{(n)}_{(ls)tri}}{R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls}}\right. \\ &-\frac{A}{5}(\delta_{tp}\delta_{ir} + \delta_{tr}\delta_{ip} + \delta_{it}\delta_{pr})\left.\left(\frac{2R_l^2\eta_l J^{(n)}_{(ll)p} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}J^{(n)}_{(ls)p}}{R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls}}\right)\right)\Bigg\} \end{aligned}$$

and again

$$\delta\omega^{(n)}_{(l)i} = 0, \tag{6.52}$$

with $N^{(n)}_{(ll)tri}$ and $N^{(n)}_{(ls)tri}$ defined in the obvious way:

$$N^{(n)}_{(ll)tri} = \frac{1}{\eta_l} \sum_{n' large} I^{(nn')}_{(ll)t} I^{(nn')}_{(ll)r} I^{(nn')}_{(ll)i} \tag{6.53}$$

and

$$N^{(n)}_{(ls)tri} = \frac{1}{\eta_{ls}} \sum_{n' small} I^{(nn')}_{(ls)t} I^{(nn')}_{(ls)r} I^{(nn')}_{(ls)i}. \tag{6.54}$$

From these approximations for the displacements, it is now possible to find expressions for the incremental forces acting across the contact area. The actual expressions found are again all very lengthy and will be omitted here. However, the methods used to find them are all identical to those already described in previous sections. From the incremental forces, the average incremental stress is found in terms of the average incremental strain and from this the effective Lamé moduli can be written down.

Next then, we need to calculate an expression for the average incremental stress and relate this to the average incremental strain. We have calculated the incremental forces acting and the general expression that relates these to this stress is given below:

$$\begin{aligned} < \delta\sigma_{ij} > \; = \; -\frac{1}{2V} & \{ N_s \eta_s R_s (< I^{(nn')}_{(ss)i} \delta F^{(nn')}_{(ss)j} > + < I^{(nn')}_{(ss)j} \delta F^{(nn')}_{(ss)i} >) \\ & + N_l \eta_l R_l (< I^{(nn')}_{(ll)i} \delta F^{(nn')}_{(ll)j} > + < I^{(nn')}_{(ll)j} \delta F^{(nn')}_{(ll)i} >) \\ & + N_s \eta_{sl} R_s (< I^{(nn')}_{(sl)i} \delta F^{(nn')}_{(sl)j} > + < I^{(nn')}_{(sl)j} \delta F^{(nn')}_{(sl)i} >) \\ & + N_l \eta_{ls} R_l (< I^{(nn')}_{(ls)i} \delta F^{(nn')}_{(ls)j} > + < I^{(nn')}_{(ls)j} \delta F^{(nn')}_{(ls)i} >) \} . \end{aligned} \tag{6.55}$$

Having substituted in the expressions for the incremental forces, we define further parameters. These are analogous to the χ introduced in Chapter 3 which was defined as:

$$\chi = \frac{1}{3} < I^{(nn')}_i I^{(nn')}_j I^{(nn')}_k N^{(n)}_{ijk} > .$$

Here we now have:

$$\chi_{ss} = \frac{1}{3} < I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} I^{(nn')}_{(ss)k} N^{(n)}_{(ss)ijk} >,$$

$$\chi_{ll} = \frac{1}{3} < I^{(nn')}_{(ll)i} I^{(nn')}_{(ll)j} I^{(nn')}_{(ll)k} N^{(n)}_{(ll)ijk} >,$$

$$\chi_{sl} = \frac{1}{3} < I^{(nn')}_{(sl)i} I^{(nn')}_{(sl)j} I^{(nn')}_{(sl)k} N^{(n)}_{(sl)ijk} >$$

and

$$\chi_{ls} = \frac{1}{3} < I^{(nn')}_{(ls)i} I^{(nn')}_{(ls)j} I^{(nn')}_{(ls)k} N^{(n)}_{(ls)ijk} > . \tag{6.56}$$

We also have some χ terms which are defined as a sum, similarly to α_{sssl} and α_{llls}, since they can again arise from two different averages. If we again let $N(s,l)\eta(s,l) = N_s(\eta_s + \eta_{sl}) + N_l(\eta_l + \eta_{ls})$, then we define

$$\chi_{sssl} = \frac{1}{3N(s,l)\eta(s,l)} \sum_n N_{(ss)ijk} N_{(sl)ijk} \tag{6.57}$$

and

$$\chi_{llls} = \frac{1}{3N(s,l)\eta(s,l)} \sum_{n} N_{(ll)ijk} N_{(ls)ijk}. \tag{6.58}$$

The parameter χ_{sssl} arises from the two average terms $< I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} I^{(nn')}_{(ss)k} N^{(n)}_{(sl)ijk} >$ and $< I^{(nn')}_{(sl)i} I^{(nn')}_{(sl)j} I^{(nn')}_{(sl)k} N^{(n)}_{(ss)ijk} >$ and we note that

$$< I^{(nn')}_{(ss)i} I^{(nn')}_{(ss)j} I^{(nn')}_{(ss)k} N^{(n)}_{(sl)ijk} >= \frac{\eta_{sl}}{3N(s,l)\eta(s,l)} \chi_{sssl}$$

and

$$< I^{(nn')}_{(sl)i} I^{(nn')}_{(sl)j} I^{(nn')}_{(sl)k} N^{(n)}_{(ss)ijk} >= \frac{\eta_{s}}{3N(s,l)\eta(s,l)} \chi_{sssl}.$$

Similarly,

$$< I^{(nn')}_{(ll)i} I^{(nn')}_{(ll)j} I^{(nn')}_{(ll)k} N^{(n)}_{(ls)ijk} >= \frac{\eta_{ls}}{3N(s,l)\eta(s,l)} \chi_{llls}$$

and

$$< I^{(nn')}_{(ls)i} I^{(nn')}_{(ls)j} I^{(nn')}_{(ls)k} N^{(n)}_{(ll)ijk} >= \frac{\eta_{l}}{3N(s,l)\eta(s,l)} \chi_{llls}.$$

These new definitions allow us to calculate the following expressions, the first of which is that for the average incremental stress. We have, $N(s,l)\eta(s,l) = N_s(\eta_s + \eta_{sl}) + N_l(\eta_l + \eta_{ls})$ and we let $R_1(s,l)\eta_1(s,l) = R_s\eta_s + (R_sR_l)^{1/2}\eta_{sl}$. Similarly, let $R_2(s,l)\eta_2(s,l) = R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls}$ and hence

$$\begin{aligned}
< \delta\sigma_{ij} > \ &= \ \frac{(-e)^{1/2}}{\pi VB(2B+C)} \left\{ \frac{1}{3N(s,l)\eta(s,l)} \left[2N_s^2\eta_s^2R_s^3 + N_l^2\eta_l^2R_l^3 \right.\right. \\
&+ (R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l) \Big] \left((B + \frac{C}{5})(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \frac{C}{5}\delta_{ij}\delta_{kl} \right) \\
&-3 \left\{ \frac{1}{R_1(s,l)\eta_1(s,l)} \left[2R_s^2N_s^2\eta_s(2R_s^2\eta_s\alpha_{ss} + (R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}\alpha_{sssl}) \right.\right. \\
&\qquad + (R_sN_s\eta_{sl} + R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_s^2\eta_s\eta_{sl}\alpha_{sssl} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl}) \Big] \\
&+ \frac{1}{R_2(s,l)\eta_2(s,l)} \left[2R_l^2N_l^2\eta_l(2R_l^2\eta_l\alpha_{ll} + (R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}\alpha_{llls}) \right. \\
&\qquad + (R_sN_s\eta_{sl} + R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_l^2\eta_l\eta_{ls}\alpha_{llls} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{sl}) \Big] \Big\} \\
&\left\{ \frac{1}{6B+C} \left[\left(2B(1-A)\left(B + \frac{2C}{5}\right) - \frac{2C^2A}{5} \right) (\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \right.\right. \\
&\qquad + \frac{C}{5}(4B(1-A) - 7CA)\delta_{ij}\delta_{kl} \Big] + A \left(\left(B + \frac{C}{5}\right)(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \frac{C}{5}\delta_{ij}\delta_{kl} \right) \Big\} \\
&- \frac{3C^2}{10(6B+C)} \left\{ \frac{1}{R_1(s,l)\eta_1(s,l)} \left[2N_s\eta_sR_s^2 \right.\right. \\
&[2R_s^2\eta_s(2(2\alpha_{ss} - \chi_{ss})\delta_{ij}\delta_{kl} + (3\chi_{ss} - \alpha_{ss})(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}))
\end{aligned}$$

$$
\begin{aligned}
&+(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}(2(2\alpha_{sssl}-\chi_{sssl})\delta_{ij}\delta_{kl}+(3\chi_{sssl}-\alpha_{sssl})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))]\\
&+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}\\
&\quad[2R_s\eta_s\eta_{sl}(2(2\alpha_{sssl}-\chi_{sssl})\delta_{ij}\delta_{kl}+(3\chi_{sssl}-\alpha_{sssl})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))\\
&\quad+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(2(2\alpha_{sl}-\chi_{sl})\delta_{ij}\delta_{kl}+(3\chi_{sl}-\alpha_{sl})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))]\Big]\\
&\qquad\qquad\left\{\frac{1}{R_2(s,l)\eta_2(s,l)}\Big[2N_l\eta_lR_l^2\right.\\
&[2R_l^2\eta_l(2(2\alpha_{ll}-\chi_{ll})\delta_{ij}\delta_{kl}+(3\chi_{ll}-\alpha_{ll})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))\\
&\quad+(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}(2(2\alpha_{llls}-\chi_{llls})\delta_{ij}\delta_{kl}+(3\chi_{llls}-\alpha_{llls})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))]\\
&+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}\\
&\quad[2R_l\eta_l\eta_{ls}(2(2\alpha_{llls}-\chi_{llsl})\delta_{ij}\delta_{kl}+(3\chi_{llls}-\alpha_{llls})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))\\
&\quad+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(2(2\alpha_{ls}-\chi_{ls})\delta_{ij}\delta_{kl}+(3\chi_{ls}-\alpha_{ls})(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}))]\Big]\Big\}\\
&+3A\left\{\frac{1}{(R_1(s,l)\eta_1(s,l))^2}\Big[2N_s\eta_sR_s^2[4R_s^3\eta_s^2\alpha_{ss}+R_l(R_s+R_l)^2\eta_s\eta_{sl}\alpha_{sl}\right.\\
&+4R_s(R_sR_l)^{1/2}\eta_s^2\eta_{sl}\alpha_{sssl}]+\frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_s^4\eta_s\eta_{sl}\alpha_{ss}\\
&\qquad\qquad+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}^2\alpha_{sssl}]\Big]\\
&+\frac{1}{(R_2(s,l)\eta_2(s,l))^2}\Big[2N_l\eta_lR_l^2[4R_l^3\eta_l^2\alpha_{ll}+R_s(R_s+R_l)^2\eta_l\eta_{ls}\alpha_{ls}\\
&+4R_l(R_sR_l)^{1/2}\eta_l^2\eta_{ls}\alpha_{llls}]+\frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_l^4\eta_l\eta_{ls}\alpha_{ll}\\
&\qquad\qquad+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}^2\alpha_{llls}]\Big]\Big\}\\
&\left\{\frac{4}{(14B+3C)}\left[\left(B+\frac{C}{5}\right)^2(\delta_{ik}\delta_{jl}+\delta_{il}\delta jk)+\frac{C}{5}\left(6B+\frac{7C}{2}\right)\delta_{ij}\delta_{kl}\right]\right.\\
&\qquad\left.-\frac{A}{2}\left(\left(B+\frac{C}{5}\right)(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})+\frac{C}{5}\delta_{ij}\delta_{kl}\right)\right\}\Big\}\,\delta e_{kl}. \qquad (6.59)
\end{aligned}
$$

Thus we have the relationship between the average incremental stress and incremental strain which allows us to calculate the effective elastic Lamé moduli for the material. The initial deformation was hydrostatic and so we have

$$< \delta\sigma_{ij} >= C^*_{ijkl} < \delta e_{kl} >$$

where

$$C^*_{ijkl} = \lambda^*\delta_{ij}\delta_{kl} + \mu^*(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}).$$

Hence, the effective Lamé moduli for a binary packing of spheres are given by

$$\begin{aligned}
\lambda^* &= \frac{C(-e)^{1/2}}{5\pi VB(2B+C)}\left\{\frac{1}{15N(s,l)\eta(s,l)}\left[2N_s^2\eta_s^2R_s^3+N_l^2\eta_l^2R_l^3\right.\right.\\
&\quad\left.+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right]\\
&-\frac{3}{5}\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\left[2R_s^2N_s^2\eta_s(2R_s^2\eta_s\alpha_{ss}+(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}\alpha_{sssl})\right.\right.\\
&\quad\left.+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_s^2\eta_s\eta_{sl}\alpha_{sssl}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl})\right]\\
&+\frac{1}{R_2(s,l)\eta_2(s,l)}\left[2R_l^2N_l^2\eta_l(2R_l^2\eta_l\alpha_{ll}+(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}\alpha_{llls})\right.\\
&\quad\left.\left.+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_l^2\eta_l\eta_{ls}\alpha_{llls}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{sl})\right]\right\}\\
&\quad\left\{\frac{1}{6B+C}[4B(1-A)-7CA)+A(6B+C)]\right\}\\
&-\frac{3C}{2(6B+C)}\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\left[2N_s\eta_sR_s^2\right.\right.\\
&\quad[4R_s^2\eta_s(2\alpha_{ss}-\chi_{ss})+2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}(2\alpha_{sssl}-\chi_{sssl})\\
&+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}\\
&\quad\left.[4R_s\eta_s\eta_{sl}(2\alpha_{sssl}-\chi_{sssl})+2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(2\alpha_{sl}-\chi_{sl})\right]\\
&\quad\left\{\frac{1}{R_2(s,l)\eta_2(s,l)}\left[2N_l\eta_lR_l^2\right.\right.\\
&\quad[4R_l^2\eta_l(2\alpha_{ll}-\chi_{ll})+2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}(2\alpha_{llls}-\chi_{llls})\\
&\quad+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}[4R_l\eta_l\eta_{ls}(2\alpha_{llls}-\chi_{llsl})\\
&\quad\left.\left.+2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(2\alpha_{ls}-\chi_{ls})\right]\right\}\\
&+3A\left\{\frac{1}{(R_1(s,l)\eta_1(s,l))^2}\left[2N_s\eta_sR_s^2[4R_s^3\eta_s^2\alpha_{ss}+R_l(R_s+R_l)^2\eta_s\eta_{sl}\alpha_{sl}\right.\right.\\
&+4R_s(R_sR_l)^{1/2}\eta_s^2\eta_{sl}\alpha_{sssl}]+\frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_s^4\eta_s\eta_{sl}\alpha_{ss}\\
&\quad\left.+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}^2\alpha_{sssl}]\right]\\
&+\frac{1}{(R_2(s,l)\eta_2(s,l))^2}\left[2N_l\eta_lR_l^2[4R_l^3\eta_l^2\alpha_{ll}+R_s(R_s+R_l)^2\eta_l\eta_{ls}\alpha_{ls}\right.\\
&+4R_l(R_sR_l)^{1/2}\eta_l^2\eta_{ls}\alpha_{llls}]+\frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_l^4\eta_l\eta_{ls}\alpha_{ll}\\
&\quad\left.\left.+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}^2\alpha_{llls}]\right]\right\}\\
&\quad\left\{\frac{4}{(14B+3C)}\left[6B+\frac{7C}{2}\right]-\frac{A}{2}\right\}\right\}\delta e_{kl} \qquad (6.60)
\end{aligned}$$

and also

$$\mu^* = \frac{(-e)^{1/2}}{\pi VB(2B+C)}\left\{\frac{1}{3N(s,l)\eta(s,l)}\left[2N_s^2\eta_s^2R_s^3+N_l^2\eta_l^2R_l^3\right.\right.$$

$$
\begin{aligned}
&\quad +(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\Big]\left(B+\frac{C}{5}\right) \\
&-3\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\Big[2R_s^2N_s^2\eta_s(2R_s^2\eta_s\alpha_{ss} + (R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}\alpha_{sssl})\right. \\
&\quad +(R_sN_s\eta_{sl} + R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_s^2\eta_s\eta_{sl}\alpha_{sssl} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl})\Big] \\
&+\frac{1}{R_2(s,l)\eta_2(s,l)}\Big[2R_l^2N_l^2\eta_l(2R_l^2\eta_l\alpha_{ll} + (R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}\alpha_{llls}) \\
&\quad \left.+(R_sN_s\eta_{sl} + R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_l^2\eta_l\eta_{ls}\alpha_{llls} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{sl})\Big]\right\} \\
&\left\{\frac{1}{6B+C}\left(2B(1-A)\left(B+\frac{2C}{5}\right) - \frac{2C^2A}{5}\right) + A\left(B+\frac{C}{5}\right)\right\} \\
&-\frac{3C^2}{10(6B+C)}\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\Big[2N_s\eta_sR_s^2\right. \\
&\qquad [2R_s^2\eta_s(3\chi_{ss}-\alpha_{ss}) + (R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}(3\chi_{sssl}-\alpha_{sssl})] \\
&+(R_sN_s\eta_{sl} + R_lN_l\eta_{ls})(R_sR_l)^{1/2} \\
&\qquad [2R_s\eta_s\eta_{sl}(3\chi_{sssl}-\alpha_{sssl}) + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(3\chi_{sl}-\alpha_{sl})] \\
&\left\{\frac{1}{R_2(s,l)\eta_2(s,l)}\Big[2N_l\eta_lR_l^2[2R_l^2\eta_l(3\chi_{ll}-\alpha_{ll}) + (R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}(3\chi_{llls}-\alpha_{llls})]\right. \\
&\quad +(R_sN_s\eta_{sl} + R_lN_l\eta_{ls})(R_sR_l)^{1/2}[2R_l\eta_l\eta_{ls}(3\chi_{llls}-\alpha_{llls}) \\
&\qquad \left.+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(3\chi_{ls}-\alpha_{ls})]\Big]\right\} \\
&+3A\left\{\frac{1}{(R_1(s,l)\eta_1(s,l))^2}\Big[2N_s\eta_sR_s^2[4R_s^3\eta_s^2\alpha_{ss} + R_l(R_s+R_l)^2\eta_s\eta_{sl}\alpha_{sl}\right. \\
&+4R_s(R_sR_l)^{1/2}\eta_s^2\eta_{sl}\alpha_{sssl}] + \frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_s^4\eta_s\eta_{sl}\alpha_{ss} \\
&\qquad +(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl} + 4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}^2\alpha_{sssl}]\Big] \\
&+\frac{1}{(R_2(s,l)\eta_2(s,l))^2}\Big[2N_l\eta_lR_l^2[4R_l^3\eta_l^2\alpha_{ll} + R_s(R_s+R_l)^2\eta_l\eta_{ls}\alpha_{ls} \\
&+4R_l(R_sR_l)^{1/2}\eta_l^2\eta_{ls}\alpha_{llls}] + \frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_l^4\eta_l\eta_{ls}\alpha_{ll} \\
&\qquad \left.+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls} + 4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}^2\alpha_{llls}]\Big]\right\} \\
&\qquad \left\{\frac{4}{(14B+3C)}\left(B+\frac{C}{5}\right)^2 - \frac{A}{2}\left(B+\frac{C}{5}\right)\right\}\delta e_{kl}.
\end{aligned} \tag{6.61}
$$

These are the new results we wished to find.

From these two moduli we can also calculate the effective bulk modulus found using $\kappa^* = \lambda^* + \frac{2}{3}\mu^*$. Thus we have

$$
\kappa^* = \frac{(-e)^{1/2}}{3\pi VB}\left\{N_s\eta_sR_s^2\left\{\frac{2N_s\eta_sR_s}{3N(s,l)\eta(s,l)}\right.\right.
$$

$$
\begin{aligned}
& -18A\left(\frac{2R_s^2\eta_s\alpha_{ss}+(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}\alpha_{sssl}}{R_1(s,l)\eta_1(s,l)}\right) \\
& +\frac{9A^2}{2R_s}\left(\frac{4R_s^4\eta_s^2\alpha_{ss}+(R_sR_l)(R_s+R_l)^2\eta_{sl}\eta_s\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\eta_s^2\alpha_{sssl}}{(R_1(s,l)\eta_1(s,l))^2}\right)\Bigg\} \\
& +N_l\eta_lR_l^2\left\{\frac{2N_l\eta_lR_l}{3N(s,l)\eta(s,l)}-18A\left(\frac{2R_l^2\eta_l\alpha_{ll}+(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}\alpha_{llls}}{R_2(s,l)\eta_2(s,l)}\right)\right. \\
& +\frac{9A^2}{2R_l}\left(\frac{4R_l^4\eta_l^2\alpha_{ll}+(R_sR_l)(R_s+R_l)^2\eta_{ls}\eta_l\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\eta_l^2\alpha_{llls}}{(R_2(s,l)\eta_2(s,l))^2}\right)\Bigg\} \\
& +(R_sN_s\eta_{sl}+R_lN_l\eta_{ls}\left\{\frac{(R_sN_s\eta_{sl}+N_l\eta_{ls}R_l)}{3N(s,l)\eta(s,l)}\right. \\
& \qquad -9A\left(\frac{2R_s^2\eta_s\eta_{sl}\alpha_{sssl}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl}}{R_1(s,l)\eta_1(s,l)}\right. \\
& \qquad\qquad \left.+\frac{2R_l^2\eta_l\eta_{ls}\alpha_{llls}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{ls}}{R_2(s,l)\eta_2(s,l)}\right) \\
& +\frac{9A^2}{2(R_s+R_l)}\left(\frac{4R_s^4\eta_s\eta_{sl}\alpha_{ss}+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}^2\eta_s\alpha_{sssl}}{(R_1(s,l)\eta_1(s,l))^2}\right. \\
& \qquad \left.\left.+\frac{4R_l^4\eta_l\eta_{ls}\alpha_{ll}+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}^2\eta_l\alpha_{llls}}{(R_2(s,l)\eta_2(s,l))^2}\right)\right\}\Bigg\}.
\end{aligned}
\tag{6.62}
$$

We check this expression for κ^* in two ways. First, we consider whether it is consistent with the initial part of the problem. If we differentiate the expression for the initial average stress, equation (6.33), then both expressions for κ^* are found to be identical. Also, if we let $R_s = R_l$, then κ^* reduces to the expression found in Chapter 3 for a packing of equal sized spheres. These are only simple checks but give us some indication as to whether our calculations are correct.

The results above again all apply only to a packing of infinitely rough spheres. If we consider instead a packing of perfectly smooth spheres then from the equations of equilibrium we find that the incremental displacement of the centre of the nth small sphere is given by:

$$
\begin{aligned}
\delta u_{(s)i}^{(n)} &= \delta e_{ij}X_{(s)i}^{(n)} \\
& -3\delta e_{rt}\left(\frac{2R_s^2\eta_sN_{(ss)tri}^{(n)}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}N_{(sl)tri}^{(n)}}{R_s\eta_s+(R_sR_l)^{1/2}\eta_{sl}}\right. \\
& \left.-\frac{1}{15}(\delta_{tp}\delta_{ir}+\delta_{tr}\delta_{ip}+\delta_{it}\delta_{pr})\left(\frac{2R_s^2\eta_sJ_{(ss)p}^{(n)}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}J_{(sl)p}^{(n)}}{R_s\eta_s+(R_sR_l)^{1/2}\eta_{sl}}\right)\right),
\end{aligned}
\tag{6.63}
$$

where all the terms are as previously defined. The rotation about an axis through its centre

$$\delta\omega^{(n)}_{(s)i} = 0. \tag{6.64}$$

Similarly, the displacement of the centre of the nth large sphere is

$$\begin{aligned}\delta u^{(n)}_{(l)i} &= \delta e_{ij} X^{(n)}_{(l)i} \\ &\quad -3\delta e_{rt}\left(\frac{2R_l^2\eta_l N^{(n)}_{(ll)tri} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}N^{(n)}_{(ls)tri}}{R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls}}\right. \\ &\quad \left.\left.-\frac{1}{15}(\delta_{tp}\delta_{ir}+\delta_{tr}\delta_{ip}+\delta_{it}\delta_{pr})\left(\frac{2R_l^2\eta_l J^{(n)}_{(ll)p} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}J^{(n)}_{(ls)p}}{R_l\eta_l + (R_sR_l)^{1/2}\eta_{ls}}\right)\right)\right\}\end{aligned} \tag{6.65}$$

and again

$$\delta\omega^{(n)}_{(l)i} = 0. \tag{6.66}$$

By substituting back we can calculate the forces acting across the contact areas from which we can then find the relationship between the average incremental stress and the incremental strain. The effective elastic Lamé moduli are calculated in the same way as above to be:

$$\begin{aligned}\lambda^* &= \frac{(-e)^{1/2}}{5\pi VB}\left\{\frac{1}{15N(s,l)\eta(s,l)}\left[2N_s^2\eta_s^2R_s^3 + N_l^2\eta_l^2R_l^3\right.\right. \\ &\quad \left.+(R_sN_s^2\eta_{sl}^2 + R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\right] \\ &-\frac{3}{5}\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\left[2R_s^2N_s^2\eta_s(2R_s^2\eta_s\alpha_{ss} + (R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}\alpha_{sssl})\right.\right. \\ &\quad \left.+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_s^2\eta_s\eta_{sl}\alpha_{sssl} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl})\right] \\ &+\frac{1}{R_2(s,l)\eta_2(s,l)}\left[2R_l^2N_l^2\eta_l(2R_l^2\eta_l\alpha_{ll} + (R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}\alpha_{llls})\right. \\ &\quad \left.\left.+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_l^2\eta_l\eta_{ls}\alpha_{llls} + (R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{sl})\right]\right\} \\ &-\frac{3}{2}\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\left[2N_s\eta_sR_s^2\right.\right. \\ &[4R_s^2\eta_s(2\alpha_{ss}-\chi_{ss}) + 2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}(2\alpha_{sssl}-\chi_{sssl}) \\ &+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2} \\ &\quad [4R_s\eta_s\eta_{sl}(2\alpha_{sssl}-\chi_{sssl}) + 2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(2\alpha_{sl}-\chi_{sl})\Big] \\ &\quad\quad \left\{\frac{1}{R_2(s,l)\eta_2(s,l)}\left[2N_l\eta_lR_l^2\right.\right. \\ &[4R_l^2\eta_l(2\alpha_{ll}-\chi_{ll}) + 2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}(2\alpha_{llls}-\chi_{llls}) \\ &+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}[4R_l\eta_l\eta_{ls}(2\alpha_{llls}-\chi_{llsl})\end{aligned}$$

$$
\begin{aligned}
&+2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(2\alpha_{ls}-\chi_{ls})\Big]\Big\}\\
&+\frac{9}{2}\left\{\frac{1}{(R_1(s,l)\eta_1(s,l))^2}\Big[2N_s\eta_sR_s^2[4R_s^3\eta_s^2\alpha_{ss}+R_l(R_s+R_l)^2\eta_s\eta_{sl}\alpha_{sl}\right.\\
&+4R_s(R_sR_l)^{1/2}\eta_s^2\eta_{sl}\alpha_{sssl}]+\frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_s^4\eta_s\eta_{sl}\alpha_{ss}\\
&\qquad+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}^2\alpha_{sssl}]\Big]\\
&+\frac{1}{(R_2(s,l)\eta_2(s,l))^2}\Big[2N_l\eta_lR_l^2[4R_l^3\eta_l^2\alpha_{ll}+R_s(R_s+R_l)^2\eta_l\eta_{ls}\alpha_{ls}\\
&+4R_l(R_sR_l)^{1/2}\eta_l^2\eta_{ls}\alpha_{llls}]+\frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_l^4\eta_l\eta_{ls}\alpha_{ll}\\
&\qquad\left.+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}^2\alpha_{llls}]\Big]\right\}\Big\}\,\delta e_{kl}
\end{aligned}
\tag{6.67}
$$

and also

$$
\begin{aligned}
\mu^* \;=\;& \frac{(-e)^{1/2}}{\pi VB}\left\{\frac{1}{15N(s,l)\eta(s,l)}\Big[2N_s^2\eta_s^2R_s^3+N_l^2\eta_l^2R_l^3\right.\\
&+(R_sN_s^2\eta_{sl}^2+R_lN_l^2\eta_{ls}^2)(R_sR_l)^{1/2}(R_s+R_l)\Big]\left(B+\frac{C}{5}\right)\\
-\frac{1}{5}&\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\Big[2R_s^2N_s^2\eta_s(2R_s^2\eta_s\alpha_{ss}+(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}\alpha_{sssl})\right.\\
&+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_s^2\eta_s\eta_{sl}\alpha_{sssl}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl})\Big]\\
+&\frac{1}{R_2(s,l)\eta_2(s,l)}\Big[2R_l^2N_l^2\eta_l(2R_l^2\eta_l\alpha_{ll}+(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}\alpha_{llls})\\
&\left.+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}(2R_l^2\eta_l\eta_{ls}\alpha_{llls}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{sl})\Big]\right\}\\
-\frac{3}{10}&\left\{\frac{1}{R_1(s,l)\eta_1(s,l)}\Big[2N_s\eta_sR_s^2\right.\\
&[2R_s^2\eta_s(3\chi_{ss}-\alpha_{ss})+(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}(3\chi_{sssl}-\alpha_{sssl})]\\
&+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}[2R_s\eta_s\eta_{sl}(3\chi_{sssl}-\alpha_{sssl})+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(3\chi_{sl}-\alpha_{sl})]\\
&\left\{\frac{1}{R_2(s,l)\eta_2(s,l)}\Big[2N_l\eta_lR_l^2[2R_l^2\eta_l(3\chi_{ll}-\alpha_{ll})+(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}(3\chi_{llls}-\alpha_{llls})]\right.\\
&+(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}[2R_l\eta_l\eta_{ls}(3\chi_{llls}-\alpha_{llls})\\
&\qquad\left.+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}(3\chi_{ls}-\alpha_{ls})]\Big]\right\}\\
+\frac{1}{50}&\left\{\frac{1}{(R_1(s,l)\eta_1(s,l))^2}\Big[2N_s\eta_sR_s^2[4R_s^3\eta_s^2\alpha_{ss}+R_l(R_s+R_l)^2\eta_s\eta_{sl}\alpha_{sl}\right.\\
&+4R_s(R_sR_l)^{1/2}\eta_s^2\eta_{sl}\alpha_{sssl}]+\frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_s^4\eta_s\eta_{sl}\alpha_{ss}\\
&\qquad+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}^2\alpha_{sssl}]\Big]\\
+&\frac{1}{(R_2(s,l)\eta_2(s,l))^2}\Big[2N_l\eta_lR_l^2[4R_l^3\eta_l^2\alpha_{ll}+R_s(R_s+R_l)^2\eta_l\eta_{ls}\alpha_{ls}
\end{aligned}
$$

$$+4R_l(R_sR_l)^{1/2}\eta_l^2\eta_{ls}\alpha_{llls}] + \frac{(R_sN_s\eta_{sl}+R_lN_l\eta_{ls})(R_sR_l)^{1/2}}{(R_s+R_l)}[4R_l^4\eta_l\eta_{ls}\alpha_{ll}$$
$$+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}^2\alpha_{llls}]\Big]\Big\}\,\delta e_{kl}. \tag{6.68}$$

From these two moduli we calculate the effective bulk modulus, $\kappa^* = \lambda^* + \frac{2}{3}\mu^*$. We find

$$\begin{aligned}
\kappa^* \;=\; & \frac{(-e)^{1/2}}{3\pi VB}\Big\{N_s\eta_sR_s^2\Big\{\frac{2N_s\eta_sR_s}{3N(s,l)\eta(s,l)} \\
& -6\left(\frac{2R_s^2\eta_s\alpha_{ss}+(R_sR_l)^{1/2}(R_s+R_l)\eta_s\eta_{sl}\alpha_{sssl}}{R_1(s,l)\eta_1(s,l)}\right) \\
& +\frac{1}{2R_s}\left(\frac{4R_s^4\eta_s^2\alpha_{ss}+(R_sR_l)(R_s+R_l)^2\eta_{sl}\eta_s\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\eta_s^2\alpha_{sssl}}{(R_1(s,l)\eta_1(s,l))^2}\right)\Big\} \\
& +N_l\eta_lR_l^2\Big\{\frac{2N_l\eta_lR_l}{3N(s,l)\eta(s,l)}-6\left(\frac{2R_l^2\eta_l\alpha_{ll}+(R_sR_l)^{1/2}(R_s+R_l)\eta_l\eta_{ls}\alpha_{llls}}{R_2(s,l)\eta_2(s,l)}\right) \\
& +\frac{1}{2R_l}\left(\frac{4R_l^4\eta_l^2\alpha_{ll}+(R_sR_l)(R_s+R_l)^2\eta_{ls}\eta_l\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\eta_l^2\alpha_{llls}}{(R_2(s,l)\eta_2(s,l))^2}\right)\Big\} \\
& +(R_sN_s\eta_{sl}+R_lN_l\eta_{ls}\Big\{\frac{(R_sN_s\eta_{sl}+N_l\eta_{ls}R_l)}{3N(s,l)\eta(s,l)} \\
& -3\left(\frac{2R_s^2\eta_s\eta_{sl}\alpha_{sssl}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}\alpha_{sl}}{R_1(s,l)\eta_1(s,l)}\right. \\
& \left.+\frac{2R_l^2\eta_l\eta_{ls}\alpha_{llls}+(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}\alpha_{ls}}{R_2(s,l)\eta_2(s,l)}\right) \\
& +\frac{1}{2(R_s+R_l)}\left(\frac{4R_s^4\eta_s\eta_{sl}\alpha_{ss}+(R_sR_l)(R_s+R_l)^2\eta_{sl}^2\alpha_{sl}+4R_s^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{sl}^2\eta_s\alpha_{sssl}}{(R_1(s,l)\eta_1(s,l))^2}\right. \\
& \left.+\frac{4R_l^4\eta_l\eta_{ls}\alpha_{ll}+(R_sR_l)(R_s+R_l)^2\eta_{ls}^2\alpha_{ls}+4R_l^2(R_sR_l)^{1/2}(R_s+R_l)\eta_{ls}^2\eta_l\alpha_{llls}}{(R_2(s,l)\eta_2(s,l))^2}\right)\Big\}\Big\}.
\end{aligned} \tag{6.69}$$

We check this by setting $\alpha = \chi = 0$ and $R_s = R_l$ when the modulus reduces to previously obtained results.

In order to compare all of these new theoretical results with those of the numerical simulations of Jenkins *et al.* [43], we must determine the values of each α and χ. The computer simulations that are used to do this are described in the next section.

6.3 The αs and χs Arising in a Binary Packing

In order to find numerical values for each α and χ defined earlier in this chapter and occurring in the expressions for the effective elastic moduli we proceed as we did in Chapter 4 when considering a packing of equal sized spheres. We wrote computer programs to simulate the spheres in contact with one and then repeated the run many times to find an average value.

In order to do these simulations, we must know the average co-ordination number of each different size of sphere. As Jenkins *et al.* [43] only discuss the co-ordination number used for a packing of equal sized spheres, we must again use the work discussed in Chapter 5, that of Dr. Luc Oger [62], to determine the value of these. We recall that he simulated a packing in which there were 16717 small spheres and 1383 large spheres, that is 92.4% of the spheres were small. This gave the average number of small spheres in contact with a typical small sphere as 4.91260 and also 0.73207 large spheres in contact with this small sphere. For a typical large sphere, there were 1.49964 other large spheres in contact with it and 8.85972 small.

As in Chapter 4, we cannot specifically calculate the values of the α and χ terms for these co-ordination numbers using our simulations. Instead, we calculate the parameter values for the two nearest whole number co-ordinations and then combine these in proportions to find an estimate of the values required. As we shall see, here we must simulate various different cases for the number of small and large spheres in contact. As was the case in Chapter 4, an especially important thing in the calculations is to impose a condition of no overlap between spheres. Also, we require equilibrium of each sphere.

The general algorithm for picking the co-ordinates of each sphere was very similar to that used for equal sized spheres. We again used the co-ordinate system (r, θ, ϕ) such that the centre of the first large sphere was at (0,0,0). Then θ and ϕ were chosen such that the centre of the first small sphere in contact with this had co-ordinates (2.7,0,0). The unit vector directed along the line of centres was then (1,0,0). A large sphere was then chosen to be in contact with the first large sphere such that $\phi = 0$, but with θ picked randomly in the interval $[0.891, \pi]$. The rest of the spheres in contact with the large were then chosen at random. These were mostly small spheres, so θ was picked in the interval $[0.759, \pi]$ to avoid overlap with the first small sphere chosen. When another large sphere was also chosen, we again pick $\theta \in [0.891, \pi]$, imposing the condition of no overlap (described later).

The program chooses a random number p say, this falls between [0,1] and so we let $\phi = 2\pi p$. In picking θ correctly, we need to ensure that the contacting spheres are distributed with an even probability density. As we have mentioned for the large spheres chosen we require θ to be contained in the interval $[0.891, \pi]$ and thus $\sin\theta \in [0.777, 1]$ or [1,0]. Similarly, for the small spheres chosen, we require $\sin\theta \in [0.688, 1]$ or [1,0] and we want the values to be chosen uniformly on these intervals. The size of the area $[\theta, \theta + \delta\theta]$ is $\sin\theta\delta\theta$ and the number of values we pick in a given area must be proportional to that area. We notice

$$\int_{\theta}^{\pi} \sin\theta d\theta = 1 + \cos\theta$$

and that

$$\int_{0.89}^{\pi} \sin\theta d\theta = 1.629$$

and

$$\int_{0.759}^{\pi} \sin\theta d\theta = 1.726.$$

From this we can see that for a large sphere we must have $1 + \cos\theta \in [0, 1.629]$ which then gives the condition $\cos\theta \in [-1, 0.629]$. Hence, to define a random θ for a large sphere we let $\theta = \cos^{-1}\{1.629q - 1\}$, where q is a second random number. Similarly, if we are trying to pick a small sphere, we must have $\cos\theta \in [-1, 0.726]$ and then let $\theta = \cos^{-1}\{1.726q - 1\}$. The unit vector $\mathbf{I}^{(nn')}$ joining the centre of the nth sphere to the n'th is found using $\mathbf{I}^{(nn')} = [\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta]$.

We must check that the current sphere does not overlap with the ones already chosen. If the unit vector joining the centre of the nth sphere to a contacting one is $\mathbf{I1} = [\sin\theta_1\cos\phi_1, \sin\theta_1\sin\phi_1, \cos\theta_1]$ and that of a second $\mathbf{I2} = [\sin\theta_2\cos\phi_2, \sin\theta_2\sin\phi_2, \cos\theta_2]$ then we must ensure that the angle separating these two is not less than $\pi/3$ for two neighbouring large spheres, $0.759rads$ for two small spheres and $0.891rads$ for neighbouring small and large spheres. We check that the cosine of the angle between them is not greater than 1/2, 0.726 and 0.629 respectively. Now, the cosine of the angle between these unit vectors is given by

$$\cos A = \sin(\theta_1)\sin(\theta_2)\cos(\theta_1 - \theta_2) + \cos(\theta_1)\cos(\theta_2),$$

we throw away this last sphere if $\cos A$ is not within the required limits. We repeat this test until the current sphere has been tested against all the other spheres. It can be very hard for the computer to find a 'gap' to put another sphere into and so if after one hundred tries it does not succeed then we throw away all the spheres chosen at this point and start again.

This process of picking random numbers and subsequently co-ordinates for the sphere centres is repeated until the required number of non-overlapping contacting spheres has been found. In this case, in order to determine all the αs and χs we must also consider a typical small sphere and so we randomly pick spheres in contact with one of the small spheres from the first part of the simulation. We chose to consider the small sphere whose centre is at (2.7,0,0) and pick the required number of small spheres in contact with this. This sphere is already in contact with one large and we do not pick anymore large spheres.

The small sphere we consider is already in contact with the initial large sphere and in order to chose random small spheres around the one in consideration and ensure no overlap with the large, we chose θ uniformly in $[0, \pi - 0.891]$. We let $\theta = \pi - \cos^{-1}\{1.629r - 1\}$, where r is a random number between 0 and 1. We must also ensure that the current small sphere does not overlap with any of those in contact chosen in the first part of the simulation. Hence, we check that the distance between the centre of the current sphere and those touching the initial large sphere is greater than or equal to 2.

We proceed to chose the rest of the spheres in the same manner as before until we have chosen the required number. At each stage we check that there is no overlap between the current sphere and the other spheres touching the small sphere and also no overlap with those from the first part of the simulation. We throw away all the spheres chosen and try again if at any point we have attempted 100 times to place a sphere and do not succeed. We also check that the small sphere is in equilibrium using the same methods as those described in Chapter 4.

The vector $\mathbf{J}$ and matrix $\mathbf{N}$ can be determined by summing components or products of the components, of the unit vectors along the line of centres between spheres. From these the values of α and χ can be calculated. A typical program is shown as an example in Appendix C.

As mentioned above, we consider different combinations of small and large spheres in contact in order to determine estimates for the α and χ terms. The average number of small spheres in contact with a particular small sphere is between 4 and 5, that for large spheres touching a small between 0 and 1. We have an average of between 1 and 2 large spheres and between 8 and 9 small spheres touching a typical large sphere. Hence we must consider the following combinations of contacts:

- 0 large and 4 small spheres in contact with a small sphere,
- 0 large and 5 small spheres in contact with a small sphere,
- 1 large and 4 small spheres in contact with a small sphere,
- 1 large and 5 small spheres in contact with a small sphere,
- 1 large and 8 small spheres in contact with a large sphere,
- 1 large and 9 small spheres in contact with a large sphere,
- 2 large and 8 small spheres in contact with a large sphere,
- 2 large and 9 small spheres in contact with a large sphere.

The table below shows the results of the calculation of the αs and χs. The combinations are abbreviated so as to be more compact, for example, $(1l4s)_s, (1l8s)_l$ represents the combination of items 3 and 5 from the list above. We notice that we have found negative values for some of the parameters. We did not find any negative values in Chapter 4, when considering equal sized spheres, but they are to be expected here. Calculation of the parameters in Chapter 4 reduced to finding the value of a squared term, for example, some multiple of $|\mathbf{J}^{(n)}|^2$ and thus, these were always positive. The parameters in this chapter cannot all be reduced in this way. Negative values arise in those parameters which consider the average over a product of two components which are related to different sized spheres in contact with the original sphere. For example, $\alpha_{sssl} = \frac{1}{3N(s,l)\eta(s,l)} \sum_n J_{(ss)i} J_{(sl)i}$, considers contact of a small sphere with both small and large spheres. For most sphere arrangements, this kind of product will consist of a combination of two components which are opposite in sign.

Parameter	$(0l4s)_s$	$(0l5s)_s$	$(1l4s)_s$, $(1l8s)_l$	$(1l5s)_s$, $(1l8s)_l$	$(1l4s)_s$, $(1l9s)_l$	$(1l5s)_s$, $(1l9s)_l$	$(1l4s)_s$, $(2l8s)_l$	$(1l5s)_s$, $(2l8s)_l$	$(1l4s)_s$, $(2l9s)_l$	$(1l5s)_s$, $(2l9s)_l$
α_{ss}	0.0153	0.0132	0.0234	0.0343	0.0211	0.0321	0.0248	0.0199	0.0239	0.0200
α_{sssl}			-0.0084	-0.0061	-0.0080	-0.0055	-0.0091	-0.0066	-0.0086	-0.0065
α_{sl}			0.0238	0.0222	0.0222	0.0208	0.0222	0.0208	0.0208	0.0196
α_{ls}			0.0085	0.0078	0.0074	0.0069	0.0095	0.0084	0.0075	0.0075
α_{llls}			-0.0029	-0.0028	-0.0027	-0.0025	-0.0024	-0.0022	-0.0021	-0.0019
α_{ll}			0.0238	0.0222	0.0222	0.0208	0.0176	0.0178	0.0172	0.0157
χ_{ss}	0.0457	0.0300	0.0236	0.0307	0.0216	0.0289	0.0237	0.0184	0.0228	0.0181
χ_{sssl}			-0.0177	-0.0165	-0.0177	-0.0143	-0.0199	-0.0191	-0.0175	-0.0184
χ_{sl}			0.0238	0.0222	0.0222	0.0208	0.0222	0.0208	0.0208	0.0196
χ_{ls}			0.0092	0.0086	0.0076	0.0071	0.0096	0.0089	0.0079	0.0085
χ_{llls}			-0.0205	-0.0184	-0.0205	-0.0195	-0.0344	-0.0321	-0.339	-0.0312
χ_{ll}			0.0238	0.0222	0.0222	0.0208	0.0190	0.0182	0.0180	0.0168

From the simulations of Dr. Oger [62] discussed in Chapter 5, we have that $\eta_s = 4.91260$, $\eta_l = 1.49964$, $\eta_{sl} = 0.73207$ and $\eta_{ls} = 8.85972$. To find an approximate value for α_{ss}, for example, we take the following combination of the results

$$\begin{aligned}\alpha_{ss} \;=\;& 0.27(0.91\alpha_{ss}(0l5s) + 0.09\alpha_{ss}(0l4s)) + 0.73\,(0.91\{0.5\,(0.86\alpha_{ss}((1l5s)_s,(1l9s)_l)\\ &+0.14\alpha_{ss}((1l5s)_s,(1l8s)_l)) + 0.5\,(0.86\alpha_{ss}((1l5s)_s,(2l9s)_l) + 0.14\alpha_{ss}((1l5s)_s,(2l8s)_l))\}\\ &+0.09\{0.5\,(0.86\alpha_{ss}((1l4s)_s,(1l9s)_l) + 0.14\alpha_{ss}((1l4s)_s,(1l8s)_l))\\ &+0.5\,(0.86\alpha_{ss}((1l4s)_s,(2l9s)_l) + 0.14\alpha_{ss}((1l4s)_s,(2l8s)_l))\}\}\,, \qquad (6.70)\end{aligned}$$

using obvious notation.

This yields a value of 0.0225 for α_{ss} and similarly the other values are found and are given in the table below. We find

α_{ss}	α_{sssl}	α_{sl}	α_{ls}	α_{llls}	α_{ll}
0.0225	-0.0046	0.0150	0.0054	-0.0016	0.0146
χ_{ss}	χ_{sssl}	χ_{sl}	χ_{ls}	χ_{llls}	χ_{ll}
0.0257	-0.0122	0.0146	0.0058	-0.0186	0.0058

Thus these approximate values for each can be substituted back into the expressions for the bulk modulus, κ^*, equation (6.62) and the shear modulus, μ^*, equation (6.61), in order to estimate the change in the values of the effective moduli. The modified values are shown in the fourth column of the table below which compares the results of this chapter with those obtained previously:

Modulus	Numerical Simulations	Walton's Theory	Theory Chapter 5	Theory Chapter 6
Bulk	185MPa	245MPa	135MPa	116MPa
Shear	127MPa	338MPa	186MPa	171MPa

The values of both moduli have decreased again. This decrease is quite large, it shows that the uniform strain approximation is not particularly good for describing a binary packing of spheres. As we mentioned before, small co-ordination numbers make the approximation inaccurate and we have dealt with a lot of small co-ordination numbers in this chapter and Chapter 5, thus we would expect there to be a large change.

Unfortunately, the bulk modulus has moved further from the value of 185MPa given by the numerical simulations, however the shear modulus has improved again, its value coming closer to the 127MPa predicted in the simulations.

6.4 Conclusions

Throughout this thesis we have tried to bring closer correlation between the predicted values of the effective elastic moduli from numerical simulations by Jenkins *et al.* [43] and those from theoretical methods. The results are all summarised in the table below:

Modulus	Numerical Simulations	Walton's Theory	Theory Chapter 3	Theory Chapter 5	Theory Chapter 6
Bulk	185MPa	245MPa	223MPa	135MPa	116MPa
Shear	127MPa	338MPa	308MPa	186MPa	171MPa

In every chapter of this thesis there has been closer correlation between the theory and simulations than there was between Walton's theory and the same simulations.

Our first modification to the theory was the work done for Chapter 3 which involved modifying the uniform strain approximation for equal sized spheres. This yielded improved predictions of the effective moduli, however the change was only around 9% for each modulus and so the correlation between the results were still not good. This is especially true of the value predicted for the shear modulus which from Walton's theory was nearly three times that of the simulations. A possible further extension of the work in Chapter 3 would be to consider some higher order terms in the perturbation of displacements and rotations of the uniform strain approximation. However, this would still not result in a significant reduction in the shear modulus as is required.

In Chapter 5, we continued by extending the uniform strain approximation to binary packings of spheres. The results were significantly different from those previously obtained by Walton and our work in Chapter 3, the shear modulus was brought much closer to the simulations. We conclude that a few large spheres amongst a packing of small can make a big difference to the properties of the packing. Since many of the co-ordination numbers used in this chapter were small, we believed that using the uniform strain approximation was alright as a first approximation but that we must again look at first order perturbations of the displacements and rotations of the sphere centres. This idea was considered in this final chapter, where more new values for the effective moduli were predicted as seen above.

The results from the theory are still not identical with those of the simulations but we have made significant progress with the work we have done. It is possible that there are other factors in the simulations that affect the results but which would be too complicated to include in the theory. In real packings and simulations, for example, each sphere does not have the same co-ordination number and this can vary greatly across the packing. When Dr. Oger [62] sent the results of his simulations and gave results for the average co-ordination numbers of small and large spheres, he also included a table which identified the exact co-ordination number for each sphere. This is shown below.

Co-ordination Number	No. of Large Spheres	No. of Small Spheres	Between Large and Large	Between Small and Small
1	0	0	527	87
2	0	0	359	533
3	15	257	131	1830
4	6	1619	16	3821
5	12	5517	1	4861
6	7	6373	34	3695
7	18	2405	21	1427
8	88	458	2	372
9	202	87	0	83
10	345	1	0	1
11	359	0	0	0
12	217	0	0	0
13	93	0	0	0
14	20	0	0	0
15	0	0	0	0
16	1	0	0	0

Then, for example, in a packing of 16717 small spheres and 1383 large spheres there are 345 large spheres with co-ordination number ten and just one small sphere with co-ordination number ten. Clearly, it would be extremely cumbersome to include these statistics into the theoretical results but it may be that this variation has an effect on the properties of the packing. We have shown how co-ordination number affects the accuracy of the uniform strain approximation in Chapter 4 when we discussed the numerical value of α which gives a measure of the deviation from ideal behaviour. For a sphere with only three or four contacts the uniform strain approximation is poor and then maybe first order perturbations are not enough. The varying co-ordination number is automatically present in the simulation.

Presented in this thesis are a few ideas which have improved the correlation between the results predicted by theory and those found using numerical simulation. We should note however, that there are still a couple of concerns that remain unanswered within the work presented. The first is the fact that in the theory, we predict values for the bulk modulus which are less than those for the shear modulus, whereas the simulations by Jenkins *et al.* [43] predict the exact opposite, that is $\mu^* < \kappa^*$. At present, the author does not have any explanation of why this might be so. The second problem that has not been addressed completely, is that of the force chains that are present in the numerical simulation sphere packings, as discussed in Cundall and Strack [25]. In Chapter 3, we mentioned how our force expressions have the scope to lead to significantly different magnitudes of force, acting on different contact areas. However, we have not been able to predict exactly how these forces vary throughout a packing. It would perhaps be interesting to address both this issue and that concerning which of the effective moduli is larger, through further work, which could involve finding out in greater detail how the packings in the numerical simulations are constructed.

Other areas for future work might include, the calculation of higher order perturbation terms, continuing the work of Chapters 3 and 6, in order to see the effect of these upon the theoretical predictions. Another interesting option could be to consider the effects of a finite coefficient of friction. In his thesis, Slade [76] considers a finite coefficient of friction for a packing of equal sized spheres. This could be extended to a binary packing, such as is discussed in Chapters 5 and 6, in order to determine the impact of friction upon, in particular, the effective elastic moduli of the packing.

Appendix A

Integral Calculations

Several integrals arise during the calculation of the effective elastic moduli upon application of an initial general biaxial strain to the boundary of our random packing. These were mentioned in Chapter 2 but details were omitted. Here we show all the integrals that arise and discuss in detail the calculation of just one, the methods for all the others being analogous.

In Chapter 2 we only mentioned the one integral

$$< (-e_{pq}I_pI_q)^{1/2}I_3^2 >\equiv \frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}\cos^2\theta\sin\theta d\theta \qquad (A.1)$$

where $e_1 < 0$ and also $e_3 < 0$. This we label integral I. In fact there are nine integrals in total that must be evaluated, the other eight are as follows:

- II.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}\sin\theta d\theta,$$
- III.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}\sin^3\theta d\theta,$$
- IV.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}\sin^5\theta d\theta,$$
- V.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1\sin^2\theta - e_3\cos^2\theta)^{1/2}\cos^2\theta\sin^3\theta d\theta,$$

- VI.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1 \sin^2\theta - e_3\cos^2\theta)^{1/2}\cos^4\theta \sin\theta d\theta,$$

- VII.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1 \sin^2\theta - e_3\cos^2\theta)^{3/2}\sin\theta d\theta,$$

- VIII.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1 \sin^2\theta - e_3\cos^2\theta)^{3/2}\cos^2\theta \sin\theta d\theta,$$

- IX.
$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1 \sin^2\theta - e_3\cos^2\theta)^{3/2}\sin^3\theta d\theta.$$

Fortunately, these do not all need to be evaluated as there are several relationships to connect them together. These are as follows:

$$\begin{aligned} I + III &= II, && \text{(A.2)}\\ IV + V &= III, && \text{(A.3)}\\ V + VI &= I, && \text{(A.4)}\\ VII &= (-e_1)III - (e_3)I, && \text{(A.5)}\\ VIII + IX &= VII, && \text{(A.6)}\\ VIII &= (-e_1)V - (e_3)VI. && \text{(A.7)} \end{aligned}$$

Re-arranging these, we also find

$$\begin{aligned} IV &= III + \frac{VIII + (e_3)I}{e_1 - e_3}, && \text{(A.8)}\\ V &= -\frac{VIII + (e_3)I}{e_1 - e_3}, && \text{(A.9)}\\ VI &= \frac{VIII + (e_3)I}{e_1 - e_3}. && \text{(A.10)} \end{aligned}$$

Hence, the values of all nine integrals can be calculated from the evaluation of just integrals I, II and VIII. We look in detail at the steps involved in the calculation of I.

We consider the calculation of integral I,

$$\frac{1}{4\pi}\int_0^{2\pi} d\phi \int_0^{\pi} (-e_1 \sin^2\theta - e_3\cos^2\theta)^{1/2}\cos^2\theta \sin\theta d\theta.$$

Calculating the integration over ϕ and splitting the interval over which we integrate with respect to θ, we have

$$I = \frac{1}{2} * 2 \int_0^{\pi/2} (-e_1 \sin^2\theta - e_3 \cos^2\theta)^{1/2} \cos^2\theta \sin\theta d\theta.$$

Now let

$$u = \cos\theta,$$

then

$$du = \sin\theta$$

and when $\theta = 0$, $u = 1$, when $\theta = \pi/2$, $u = 0$. Thus we have

$$\begin{aligned} I &= \int_1^0 -(-e_1(1-u^2) - e_3u^2)^{1/2}u^2 du \\ &= \int_0^1 (-e_1(1-u^2) - e_3u^2)^{1/2}u^2 du. \end{aligned}$$

We also let $f_1 = -e_1$ and $f_3 = -e_3$, so that

$$I = \int_0^1 (f_1 + (f_3 - f_1)u^2)^{1/2} u^2 du. \tag{A.11}$$

We must consider the two cases $f_1 > f_3$ and $f_3 < f_1$ seperately.

For the first case $f_1 > f_3$, we introduce the further substitution

$$(f_1 - f_3)^{1/2} u = f_1^{1/2} \sin\Theta,$$

so then

$$(f_1 - f_3)^{1/2} du = f_1^{1/2} \cos\Theta d\Theta.$$

This gives us:

$$I = \int_0^{\Theta_0} (\frac{f_1}{(f_1 - f_3)})^{3/2} [f_1 - f_1 \sin^2\Theta]^{1/2} \sin^2\Theta \cos\Theta d\Theta$$

where

$$\sin\Theta_0 = (\frac{(f_1 - f_3)}{f_1})^{1/2}.$$

Thus

$$I = \frac{f_1^2}{(f_1 - f_3)^{3/2}} \int_0^{\Theta_0} \sin^2 \Theta \cos^2 \Theta d\Theta.$$

This can be evaluated using the identities

$$\sin 2\Theta = 2 \sin \Theta \cos \Theta$$

and

$$1 - \cos 4\Theta = 2 \sin^2 2\Theta$$

so that

$$I = \frac{f_1^2}{8(f_1 - f_3)^{3/2}} \left[\Theta - \frac{\sin 4\Theta}{4} \right]_0^{\Theta_0}.$$

So, for $-e_1 > -e_3 > 0$. the integral is evaluated to be:

$$I = \frac{(-e_1)^2}{8(e_3 - e_1)^{3/2}} \left\{ \sin^{-1} \left(\frac{e_1 - e_3}{e_1} \right)^{1/2} + \frac{(e_3 - e_1)^{1/2}}{e_1^2} (-e_3)^{1/2} (2e_3 - e_1) \right\}. \quad \text{(A.12)}$$

Considering now the case when $f_3 > f_1$ i.e. $-e_3 > -e_1$ we proceed in a similar manner. Recalling equation (A.11), we have reduced integral I to:

$$I = \int_0^1 (f_1 + (f_3 - f_1)u^2)^{1/2} u^2 du.$$

We let

$$(f_3 - f_1)^{1/2} u = f_1^{1/2} \sinh \Theta$$

and then

$$(f_3 - f_1)^{1/2} du = f_1^{1/2} \cosh \Theta d\Theta.$$

So the integral becomes

$$I = \int_0^{\Theta_0} (\frac{f_1}{(f_3 - f_1)})^{3/2} [f_1 + f_1 \sinh^2 \Theta]^{1/2} \sinh^2 \Theta \cosh \Theta d\Theta$$

where Θ_0 is now found from

$$\sinh \Theta_0 = (\frac{(f_3 - f_1)}{f_1})^{1/2}.$$

So we have

$$I = \frac{f_1^2}{(f_3 - f_1)^{3/2}} \int_0^{\Theta_0} \sinh^2 \Theta \cosh^2 \Theta d\Theta.$$

This can be evaluated using the identities

$$\sinh 2\Theta = 2 \sinh \Theta \cosh \Theta$$

and

$$\cosh 4\Theta - 1 = 2 \sinh^2 2\Theta$$

so that

$$I = \frac{f_1^2}{8(f_3 - f_3)^{3/2}} \left[\Theta - \frac{\sin 4\Theta}{4}\right]_0^{\Theta_0}.$$

So, for $-e_3 > -e_1 > 0$. integral I is evaluated as:

$$I = \frac{(-e_1)^2}{8(e_1 - e_3)^{3/2}} \left\{ \frac{(e_1 - e_3)^{1/2}}{e_1^2} (-e_3)^{1/2} (e_1 - 2e_3) - \sinh^{-1} \left(\frac{e_3 - e_1}{e_1} \right)^{1/2} \right\}. \quad \text{(A.13)}$$

If it were required, all the other integrals could be calculated in a similar manner.

Appendix B

Calculation of α and χ for different sized spheres

Computer program used to calculate the values of α and χ for a binary packing, from an initial large and small sphere in contact with each other. The large sphere is further surrounded by one large and eight small spheres and the original small sphere is surrounded by a further four small spheres. Both of the original spheres are in equilibrium.

```
function y = diffsp1814()

g=100; h=100; i=100; j=100; k=100; l=100;
while g==100 | h==100 | i==100 | j==100 | k==100 | l==100

clear

a1=0;
b1=0;
I1=[0; 0; 1];  %this represents a small sphere touching the large one
m2=rand;
a2 = acos(1.629*m2 - 1); %pick large sphere next
b2=0;
I2=[sin(a2)*cos(b2); sin(a2)*sin(b2); cos(a2)];
K2=[3.4*sin(a2)*cos(b2); 3.4*sin(a2)*sin(b2); 3.4*cos(a2)-1.7];

B1=3/4; B2=3/4; B3=3/4;
B4=3/4; B5=3/4; B6=3/4;
B7=3/4; B8=3/4; B9=3/4;
B10=3/4; B11=3/4; B12=3/4;
B13=3/4; B14=3/4; B15=3/4;
B16=3/4; B17=3/4; B18=3/4;
B19=3/4; B20=3/4; B21=3/4;
B22=3/4; B23=3/4; B24=3/4;
B25=3/4; B26=3/4;
B27=3/4; B28=3/4;
```

```
%now pick another 7 small spheres, not overlapping with the previously
%chosen spheres
while B1>0.629          %check small sphere doesn't overlap with large
m3=rand;
a3 = acos(3*m3/2 - 1);
b3=2*pi*rand;
B1=sin(a2)*sin(a3)*cos(b2-b3) +cos(a2)*cos(a3);
I3=[sin(a3)*cos(b3); sin(a3)*sin(b3); cos(a3)];
K3=[2.7*sin(a3)*cos(b3); 2.7*sin(a3)*sin(b3); 2.7*cos(a3)-1.7];
end;            %end of while B1>0.629 loop

while B2>0.629 | B3>0.726
%check sphere doesn't overlap with those already chosen
m4=rand;
a4 = acos(3*m4/2 - 1);
b4=2*pi*rand;
B2=sin(a2)*sin(a4)*cos(b2-b4) +cos(a2)*cos(a4);
B3=sin(a3)*sin(a4)*cos(b3-b4) +cos(a3)*cos(a4);
I4=[sin(a4)*cos(b4); sin(a4)*sin(b4); cos(a4)];
K4=[2.7*sin(a4)*cos(b4); 2.7*sin(a4)*sin(b4); 2.7*cos(a4)-1.7];
end;            %end of while B2>0.629 | B3>0.5 loop

while B4>0.629 | B5>0.726 | B6>0.726
m5=rand;
a5 = acos(3*m5/2 - 1);
b5=2*pi*rand;
B4=sin(a2)*sin(a5)*cos(b2-b5) +cos(a2)*cos(a5);
B5=sin(a3)*sin(a5)*cos(b3-b5) +cos(a3)*cos(a5);
B6=sin(a4)*sin(a5)*cos(b4-b5) +cos(a4)*cos(a5);
I5=[sin(a5)*cos(b5); sin(a5)*sin(b5); cos(a5)];
K5=[2.7*sin(a5)*cos(b5); 2.7*sin(a5)*sin(b5); 2.7*cos(a5)-1.7];
end;            %end of while B4>0.629 | B5>0.5 | B6>0.5

while B7>0.629 | B8>0.726 | B9>0.726 | B10>0.726
m6=rand;
a6 = acos(3*m6/2 - 1);
b6=2*pi*rand;
B7=sin(a2)*sin(a6)*cos(b2-b6) +cos(a2)*cos(a6);
B8=sin(a3)*sin(a6)*cos(b3-b6) +cos(a3)*cos(a6);
B9=sin(a4)*sin(a6)*cos(b4-b6) +cos(a4)*cos(a6);
B10=sin(a5)*sin(a6)*cos(b5-b6) +cos(a5)*cos(a6);
I6=[sin(a6)*cos(b6); sin(a6)*sin(b6); cos(a6)];
K6=[2.7*sin(a6)*cos(b6); 2.7*sin(a6)*sin(b6); 2.7*cos(a6)-1.7];
end;            %end of while B7>0.629 etc loop

while B11>0.629 | B12>0.726 | B13>0.726 | B14>0.726 | B15>0.726
m7=rand;
a7 = acos(3*m7/2 - 1);
b7=2*pi*rand;
B11=sin(a2)*sin(a7)*cos(b2-b7) +cos(a2)*cos(a7);
B12=sin(a3)*sin(a7)*cos(b3-b7) +cos(a3)*cos(a7);
B13=sin(a4)*sin(a7)*cos(b4-b7) +cos(a4)*cos(a7);
B14=sin(a5)*sin(a7)*cos(b5-b7) +cos(a5)*cos(a7);
B15=sin(a6)*sin(a7)*cos(b6-b7) +cos(a6)*cos(a7);
I7=[sin(a7)*cos(b7); sin(a7)*sin(b7); cos(a7)];
K7=[2.7*sin(a7)*cos(b7); 2.7*sin(a7)*sin(b7); 2.7*cos(a7)-1.7];
end;            %end of while B11>0.629 etc. loop

g=0; h=0; i=0; j=0; k=0; l=0;

while B16>0.629|B17>0.726|B18>0.726|B19>0.726|B20>0.726|B21>0.726 & g<100
m8=rand;
g=g+1;
a8 = acos(3*m8/2 - 1);
```

```
b8=2*pi*rand;
B16=sin(a2)*sin(a8)*cos(b2-b8) +cos(a2)*cos(a8);
B17=sin(a3)*sin(a8)*cos(b3-b8) +cos(a3)*cos(a8);
B18=sin(a4)*sin(a8)*cos(b4-b8) +cos(a4)*cos(a8);
B19=sin(a5)*sin(a8)*cos(b5-b8) +cos(a5)*cos(a8);
B20=sin(a6)*sin(a8)*cos(b6-b8) +cos(a6)*cos(a8);
B21=sin(a7)*sin(a8)*cos(b7-b8) +cos(a7)*cos(a8);
I8=[sin(a8)*cos(b8); sin(a8)*sin(b8); cos(a8)];
K8=[2.7*sin(a8)*cos(b8); 2.7*sin(a8)*sin(b8); 2.7*cos(a8)-1.7];
end;            %end of while B16>0.629 etc. loop

if g~=100
while B22>0.629|B23>0.726|B24>0.726|B25>0.726|B26>0.726|B27>0.726|B28>0.726&h<100

h=h+1;
m9=rand;
a9= acos(3*m9/2 - 1);
b9=2*pi*rand;
B22=sin(a2)*sin(a9)*cos(b2-b9) +cos(a2)*cos(a9);
B23=sin(a3)*sin(a9)*cos(b3-b9) +cos(a3)*cos(a9);
B24=sin(a4)*sin(a9)*cos(b4-b9) +cos(a4)*cos(a9);
B25=sin(a5)*sin(a9)*cos(b5-b9) +cos(a5)*cos(a9);
B26=sin(a6)*sin(a9)*cos(b6-b9) +cos(a6)*cos(a9);
B27=sin(a7)*sin(a9)*cos(b7-b9) +cos(a7)*cos(a9);
B28=sin(a8)*sin(a9)*cos(b8-b9) +cos(a8)*cos(a9);
I9=[sin(a9)*cos(b9); sin(a9)*sin(b9); cos(a9)];
K9=[2.7*sin(a9)*cos(b9); 2.7*sin(a9)*sin(b9); 2.7*cos(a9)-1.7];
end;            %end of B22>0.629 etc. loop


if h~=100
n=-1;
while n==-1
a21=0;
b22=0;
I10=[0; 0; -1];

k1=1; k2=1; k3=1; k4=1; k5=1; k6=1; k7=1; k8=1;
while k1<2.70 | k2<2 | k3<2 | k4<2 | k5<2 | k6<2 | k7<2 | k8<2 & i<100
i=i+1;
m11=rand;
a11 = pi - acos(1.629*m11 - 1); %pick small spheres such that they don't
%overlap with large
b11 = 2*pi*rand;
I11=[sin(a11)*cos(b11); sin(a11)*sin(b11); cos(a11)];
K11=[2*sin(a11)*cos(b11); 2*sin(a11)*sin(b11); 2*cos(a11)+1];
k1 = norm(K11-K2);
k2 = norm(K11-K3);
k3 = norm(K11-K4);
k4 = norm(K11-K5);
k5 = norm(K11-K6);
k6 = norm(K11-K7);
k7 = norm(K11-K8);
k8 = norm(K11-K9);
end             %end of while k1<2.70 etc. loop


B29=3/4; B30=3/4; B31=3/4; B32=3/4; B33=3/4; B34=3/4;
k9=1; k10=1; k11=1; k12=1; k13=1; k14=1; k15=1; k16=1;
if i~=100
while k9<2.70| k10<2| k11<2| k12<2| k13<2| k14<2| k15<2| k16<2| B29>0.5 &j<100
j=j+1;
m12 =rand;
a12 = pi - acos(1.629*m12 - 1);
```

```
b12 =2*pi*rand;
B29=sin(a11)*sin(a12)*cos(b11-b12) +cos(a11)*cos(a12);
I12=[sin(a12)*cos(b12); sin(a12)*sin(b12); cos(a12)];
K12=[2*sin(a12)*cos(b12); 2*sin(a12)*sin(b12); 2*cos(a12)+1];
k9 = norm(K12-K2);
k10 = norm(K12-K3);
k11 = norm(K12-K4);
k12 = norm(K12-K5);
k13 = norm(K12-K6);
k14 = norm(K12-K7);
k15 = norm(K12-K8);
k16 = norm(K12-K9);
end;            %end of while k9<2.70 loop

k17=1; k18=1; k19=1; k20=1; k21=1; k22=1; k23=1; k24=1;
if j~=100
while k17<2.70|k18<2|k19<2|k20<2|k21<2|k22<2|k23<2|k24<2|B30>0.5|B31>0.5&k<100
k=k+1;
m13=rand;
a13= pi - acos(1.629*m13 - 1);
b13 =2*pi*rand;
B30=sin(a11)*sin(a13)*cos(b11-b13) +cos(a11)*cos(a13);
B31=sin(a12)*sin(a13)*cos(b12-b13) +cos(a12)*cos(a13);
I13=[sin(a13)*cos(b13); sin(a13)*sin(b13); cos(a13)];
K13=[2*sin(a13)*cos(b13); 2*sin(a13)*sin(b13); 2*cos(a13)+1];
k17 = norm(K13-K2);
k18 = norm(K13-K3);
k19 = norm(K13-K4);
k20 = norm(K13-K5);
k21 = norm(K13-K6);
k22 = norm(K13-K7);
k23 = norm(K13-K8);
k24 = norm(K13-K9);
end; %end of while while k17<2.70


k25=1; k26=1; k27=1; k28=1; k29=1; k30=1; k31=1; k32=1; k33=1;
if k~=100
while k25<2.70|k26<2|k27<2|k28<2|k29<2|k30<2|k31<2|k32<2|B32>0.5|B33>0.5|B34<0.5&l<100
l=l+1;
m14=rand;
a14= pi - acos(1.629*m14 - 1);
b14 =2*pi*rand;
B32=sin(a11)*sin(a14)*cos(b11-b14) +cos(a11)*cos(a14);
B33=sin(a12)*sin(a14)*cos(b12-b14) +cos(a12)*cos(a14);
B34=sin(a13)*sin(a14)*cos(b13-b14) +cos(a13)*cos(a14);
I14=[sin(a14)*cos(b14); sin(a14)*sin(b14); cos(a14)];
K14=[2*sin(a14)*cos(b14); 2*sin(a14)*sin(b14); 2*cos(a14)+1];
k25 = norm(K14-K2);
k26 = norm(K14-K3);
k27 = norm(K14-K4);
k28 = norm(K14-K5);
k29 = norm(K14-K6);
k30 = norm(K14-K7);
k31 = norm(K14-K8);
k32 = norm(K14-K9);
end;
end;

c01 = cross(I10,I11);
c02 = cross(I10,I12);
c03 = cross(I10,I13);
c04 = cross(I10,I14);
c12 = cross(I11,I12);
```

```
c13 = cross(I11,I13);
c14 = cross(I11,I14);
c23 = cross(I12,I13);
c24 = cross(I12,I14);
c34 = cross(I13,I14);

d012 = c01'*I12;
d013 = c01'*I13;
d014 = c01'*I14;
d023 = c02'*I13;
d024 = c02'*I14;
d034 = c03'*I14;
d123 = c12'*I13;
d124 = c12'*I14;
d134 = c13'*I14;
d234 = c23'*I14;

s(1,1)=0;
s(2,2)=0;
s(3,3)=0;
s(4,4)=0;
s(5,5)=0;
s(4,5)=sign(d012);
s(3,5)=sign(d013);
s(3,4)=sign(d014);
s(2,5)=sign(d023);
s(2,4)=sign(d024);
s(2,3)=sign(d034);
s(1,5)=sign(d123);
s(1,4)=sign(d124);
s(1,3)=sign(d134);
s(1,2)=sign(d234);


if s(1,5)*s(2,5)<0 & s(1,5)*s(3,5)>0 & s(2,5)*s(4,5)>0
n=1;
m=5;
elseif s(1,2)*s(1,3)<0 & s(1,2)*s(1,4)>0 & s(1,3)*s(1,5)>0
n=1;
m=1;
elseif s(1,2)*s(2,3)<0 & s(1,2)*s(2,4)>0 & s(2,3)*s(2,5)>0
n=1;
m=2;
elseif s(1,3)*s(2,3)<0 & s(1,3)*s(3,4)>0 & s(2,3)*s(3,5)>0
n=1;
m=3;
elseif s(1,4)*s(2,4)<0 & s(1,4)*s(3,4)>0 & s(2,4)*s(4,5)>0
n=1;
m=4;
else n=-1;
m=6;

end %end of if s(1,5)*s(2,5)<0 loop


end    %end of if k~=100 loop
end    %end of if j~=100 loop
end    %end of if i~=100 loop

end    %end of while n==-1

end    %end of if h~=100 loop
end    %end of if g~=100 loop
```

```
if l~=100 & l~=0
Jls=(I1+I3+I4+I5+I6+I7+I8+I9)/8;
Jll=I2;

Jss=(I11+I12+I13+I14)/4;
Jsl=I10;

%N= N_s(eta_s+eta_sl) + N_l(eta_l+eta_ls) = 1*(4+1) + 1*(1+8) = 14

alpha_ns  =4*Jss'*Jss/42;
alpha_sssl =Jss'*Jsl/42;
%xi_sssl   =Jss'*Jsl/42;
%xi_ssll   =Jss'*Jll/42;
alpha_nsl =1*Jsl'*Jsl/42;
%xi_lssl   =Jls'*Jsl/42;
%xi_lsll   =Jls'*Jll/42;
alpha_nls =8*Jls'*Jls/42;
alpha_lsll=Jls'*Jll/42;
alpha_nl  =1*Jll'*Jll/42;

I1111=0;
I1112=0;
I1113=0;
I1122=0;
I1123=0;
I1133=0;
I1222=0;
I1223=0;
I1233=0;
I1333=1;

I2111=I2(1)^3;
I2112=I2(1)^2*I2(2);
I2113=I2(1)^2*I2(3);
I2122=I2(1)*I2(2)^2;
I2123=I2(1)*I2(2)*I2(3);
I2133=I2(1)*I2(3)^2;
I2222=I2(2)^3;
I2223=I2(2)^2*I2(3);
I2233=I2(2)*I2(3)^2;
I2333=I2(3)^3;

I3111=I3(1)^3;
I3112=I3(1)^2*I3(2);
I3113=I3(1)^2*I3(3);
I3122=I3(1)*I3(2)^2;
I3123=I3(1)*I3(2)*I3(3);
I3133=I3(1)*I3(3)^2;
I3222=I3(2)^3;
I3223=I3(2)^2*I3(3);
I3233=I3(2)*I3(3)^2;
I3333=I3(3)^3;

I4111=I4(1)^3;
I4112=I4(1)^2*I4(2);
I4113=I4(1)^2*I4(3);
I4122=I4(1)*I4(2)^2;
I4123=I4(1)*I4(2)*I4(3);
I4133=I4(1)*I4(3)^2;
I4222=I4(2)^3;
I4223=I4(2)^2*I4(3);
I4233=I4(2)*I4(3)^2;
I4333=I4(3)^3;
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```
I5111=I5(1)^3;
I5112=I5(1)^2*I5(2);
I5113=I5(1)^2*I5(3);
I5122=I5(1)*I5(2)^2;
I5123=I5(1)*I5(2)*I5(3);
I5133=I5(1)*I5(3)^2;
I5222=I5(2)^3;
I5223=I5(2)^2*I5(3);
I5233=I5(2)*I5(3)^2;
I5333=I5(3)^3;

I6111=I6(1)^3;
I6112=I6(1)^2*I6(2);
I6113=I6(1)^2*I6(3);
I6122=I6(1)*I6(2)^2;
I6123=I6(1)*I6(2)*I6(3);
I6133=I6(1)*I6(3)^2;
I6222=I6(2)^3;
I6223=I6(2)^2*I6(3);
I6233=I6(2)*I6(3)^2;
I6333=I6(3)^3;

I7111=I7(1)^3;
I7112=I7(1)^2*I7(2);
I7113=I7(1)^2*I7(3);
I7122=I7(1)*I7(2)^2;
I7123=I7(1)*I7(2)*I7(3);
I7133=I7(1)*I7(3)^2;
I7222=I7(2)^3;
I7223=I7(2)^2*I7(3);
I7233=I7(2)*I7(3)^2;
I7333=I7(3)^3;

I8111=I8(1)^3;
I8112=I8(1)^2*I8(2);
I8113=I8(1)^2*I8(3);
I8122=I8(1)*I8(2)^2;
I8123=I8(1)*I8(2)*I8(3);
I8133=I8(1)*I8(3)^2;
I8222=I8(2)^3;
I8223=I8(2)^2*I8(3);
I8233=I8(2)*I8(3)^2;
I8333=I8(3)^3;

I9111=I9(1)^3;
I9112=I9(1)^2*I9(2);
I9113=I9(1)^2*I9(3);
I9122=I9(1)*I9(2)^2;
I9123=I9(1)*I9(2)*I9(3);
I9133=I9(1)*I9(3)^2;
I9222=I9(2)^3;
I9223=I9(2)^2*I9(3);
I9233=I9(2)*I9(3)^2;
I9333=I9(3)^3;

I10111=I10(1)^3;
I10112=I10(1)^2*I10(2);
I10113=I10(1)^2*I10(3);
I10122=I10(1)*I10(2)^2;
I10123=I10(1)*I10(2)*I10(3);
I10133=I10(1)*I10(3)^2;
I10222=I10(2)^3;
I10223=I10(2)^2*I10(3);
I10233=I10(2)*I10(3)^2;
```

```
I10333=I10(3)^3;

I11111=I11(1)^3;
I11112=I11(1)^2*I11(2);
I11113=I11(1)^2*I11(3);
I11122=I11(1)*I11(2)^2;
I11123=I11(1)*I11(2)*I11(3);
I11133=I11(1)*I11(3)^2;
I11222=I11(2)^3;
I11223=I11(2)^2*I11(3);
I11233=I11(2)*I11(3)^2;
I11333=I11(3)^3;

I12111=I12(1)^3;
I12112=I12(1)^2*I12(2);
I12113=I12(1)^2*I12(3);
I12122=I12(1)*I12(2)^2;
I12123=I12(1)*I12(2)*I12(3);
I12133=I12(1)*I12(3)^2;
I12222=I12(2)^3;
I12223=I12(2)^2*I12(3);
I12233=I12(2)*I12(3)^2;
I12333=I12(3)^3;

I13111=I13(1)^3;
I13112=I13(1)^2*I13(2);
I13113=I13(1)^2*I13(3);
I13122=I13(1)*I13(2)^2;
I13123=I13(1)*I13(2)*I13(3);
I13133=I13(1)*I13(3)^2;
I13222=I13(2)^3;
I13223=I13(2)^2*I13(3);
I13233=I13(2)*I13(3)^2;
I13333=I13(3)^3;

I14111=I14(1)^3;
I14112=I14(1)^2*I14(2);
I14113=I14(1)^2*I14(3);
I14122=I14(1)*I14(2)^2;
I14123=I14(1)*I14(2)*I14(3);
I14133=I14(1)*I14(3)^2;
I14222=I14(2)^3;
I14223=I14(2)^2*I14(3);
I14233=I14(2)*I14(3)^2;
I14333=I14(3)^3;


Ns111  =I11111+I12111+I13111+I14111;
Nsl111 =I10111;
Nl111  =I2111;
Nls111 =I1111+I3111+I4111+I5111+I6111+I7111+I8111+I9111;

Ns112  =I11112+I12112+I13112+I14112;
Nsl112 =I10112;
Nl112  =I2112;
Nls112  =I1112+I3112+I4112+I5112+I6112+I7112+I8112+I9112;

Ns113  =I11113+I12113+I13113+I14113;
Nsl113 =I10113;
Nl113  =I2113;
Nls113 =I1113+I3113+I4113+I5113+I6113+I7113+I8113+I9113;

Ns122  =I11122+I12122+I13122+I14122;
Nsl122 =I10122;
```

```
Nl122  =I2122;
Nls122 =I1122+I3122+I4122+I5122+I6122+I7122+I8122+I9122;

Ns123  =I11123+I12123+I13123+I14123;
Nsl123 =I10123;
Nl123  =I2123;
Nls123 =I1123+I3123+I4123+I5123+I6123+I7123+I8123+I9123;

Ns133  =I11133+I12133+I13133+I14133;
Nsl133 =I10133;
Nl133  =I2133;
Nls133 =I1133+I3133+I4133+I5133+I6133+I7133+I8133+I9133;

Ns222  =I11222+I12222+I13222+I14222;
Nsl222 =I10222;
Nl222  =I2222;
Nls222 =I1222+I3222+I4222+I5222+I6222+I7222+I8222+I9222;

Ns223  =I11223+I12223+I13223+I14223;
Nsl223 =I10223;
Nl223  =I2223;
Nls223 =I1223+I3223+I4223+I5223+I6223+I7223+I8223+I9223;

Ns233  =I11233+I12233+I13233+I14233;
Nsl233 =I10233;
Nl233  =I2233;
Nls233 =I1233+I3233+I4233+I5233+I6233+I7233+I8233+I9233;

Ns333  =I11333+I12333+I13333+I14333;
Nsl333 =I10333;
Nl333  =I2333;
Nls333 =I1333+I3333+I4333+I5333+I6333+I7333+I8333+I9333;

Ns=Ns111^2+3*(Ns112^2)+3*(Ns113^2)+3*(Ns122^2)+6*(Ns123^2)+3*(Ns133^2)
+Ns222^2+3*(Ns223^2)+3*(Ns233^2)+Ns333^2;
Nsl=Nsl111^2+3*(Nsl112^2)+3*(Nsl113^2)+3*(Nsl122^2)+6*(Nsl123^2)+3*(Nsl133^2)
+Nsl222^2+3*(Nsl223^2)+3*(Nsl233^2)+Nsl333^2;
Nl=Nl111^2+3*(Nl112^2)+3*(Nl113^2)+3*(Nl122^2)+6*(Nl123^2)+3*(Nl133^2)
+Nl222^2+3*(Nl223^2)+3*(Nl233^2)+Nl333^2;
Nls=Nls111^2+3*(Nls112^2)+3*(Nls113^2)+3*(Nls122^2)+6*(Nls123^2)+3*(Nls133^2)
+Nls222^2+3*(Nls223^2)+3*(Nls233^2)+Nls333^2;
Nssl=Ns111*Nsl111+3*Ns112*Nsl112+3*Ns113*Nsl113+3*Ns122*Nsl122+6*Ns123*Nsl123
+3*Ns133*Nsl133+Ns222*Nsl222+3*Ns223*Nsl223+3*Ns233*Nsl223+Ns333*Nsl333;
Nlsl1=Nls111*Nl111+3*Nls112*Nl112+3*Nls113*Nl113+3*Nls122*Nl122+6*Nls123*Nl123
+3*Nls133*Nl133+Nls222*Nl222+3*Nls223*Nl223+3*Nls233*Nl223+Nls333*Nl333;

Cs=Ns/(4*42);
Csl=Nsl/(1*42);
Cl=Nl/42;
Cls=Nls/(8*42);
Cssl=Nssl/42;
Clsl1=Nlsl1/42;

y=[alpha_ns,alpha_sssl,alpha_nsl,alpha_nls,alpha_lsl1,alpha_nl,Cs,Cssl,Csl,Cls,Clsl1,Cl];

end     %end of if l~=100 & l~=0 loop


end     %end of while g==100 | h==100 | i==100 | j==100 | k==100 | l==100 loop
```

Appendix C

Table of Isotropic Elastic Constants

	λ, μ	μ, ν	E, ν	B, C
λ	λ	$\frac{2\mu\nu}{(1-2\nu)}$	$\frac{E\nu}{(1+\nu)(1-2\nu)}$	$\frac{C}{\pi(B^2-C^2)}$
μ	μ	μ	$\frac{E}{2(1+\nu)}$	$\frac{1}{2\pi(B+C)}$
κ	$\lambda + \frac{2}{3}\mu$	$\frac{2\mu(1+\nu)}{3(1-2\nu)}$	$\frac{E}{3(1-2\nu)}$	$\frac{2B+C}{3\pi(B^2-C^2)}$
E	$\frac{\mu(3\lambda+2\mu)}{\lambda+\mu}$	$2\nu(1+\nu)$	E	$\frac{B+2C}{\pi(B+C)}$
ν	$\frac{\lambda}{2(\lambda+\mu)}$	ν	ν	$\frac{C}{B+C}$
B	$\frac{1}{4\pi}\left(\frac{1}{\mu} + \frac{1}{\lambda+\mu}\right)$	$\frac{(1-\nu)}{2\pi\mu}$	$\frac{1-\nu^2}{\pi E}$	B
C	$\frac{1}{4\pi}\left(\frac{1}{\mu} - \frac{1}{\lambda+\mu}\right)$	$\frac{\nu}{2\pi\mu}$	$\frac{\nu(1+\nu)}{\pi E}$	C

λ and μ are the Lamé moduli, κ the bulk modulus, E is Young's modulus and ν Poisson's ratio.

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